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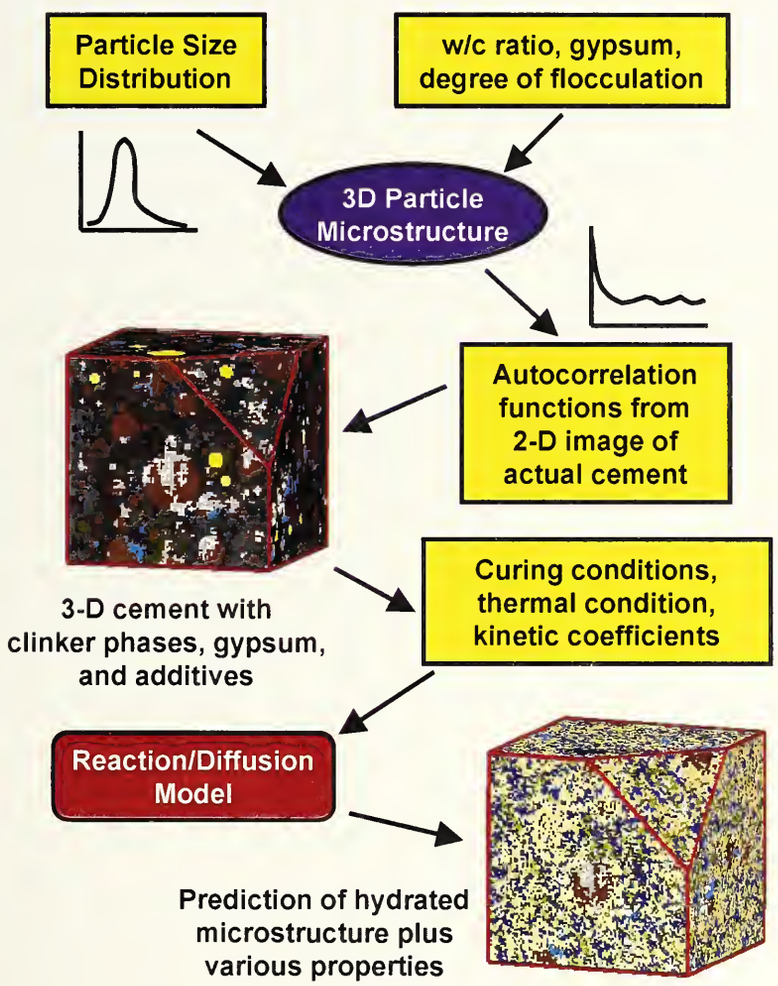
User's Guide to the Virtual Cement and Concrete Testing Laboratory



Version 1.1

Jeffrey W. Bullard

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User's Guide to the Virtual Cement and Concrete Testing Laboratory

Version 1.1

Jeffrey W. Bullard
Building and Fire Research Laboratory
National Institute of Standards and Technology

March 2003

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User's Guide to the
Virtual Cement and Concrete Testing Laboratory
Version 1.1

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ABSTRACT

This document serves as the user's manual for Version 1.1 of the Virtual Cement and Concrete Testing Laboratory (VCCTL). Using the VCCTL, a user may create starting microstructures of cement (gypsum, fly ash, etc.) particles in water, hydrate the microstructures under controlled curing conditions, leach the portlandite and remaining cement clinker phases from hydrated microstructures, subject hydrated microstructures to attack by sulfate solutions, view images and animations of 3-D microstructures, and/or evaluate a variety of properties of hydrated/leached microstructures for direct comparison to experimental data. The VCCTL includes a web-based interface that provides a menu-driven system of forms for obtaining user input and returning results.

Keywords: Building technology, cement hydration, computer modeling, concrete testing, microstructure, simulation, virtual laboratory.

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1 Introduction

This user's manual provides guidance for using Version 1.1 of the Virtual Cement and Concrete Testing Laboratory (VCCTL). This virtual laboratory consists of a web-based interface and underlying computer models and programs that allow users to create, hydrate, degrade, and evaluate 3-D cement-based microstructures from a desktop computer. Thus, the VCCTL should serve the cement and concrete research and development community, ultimately reducing the number of costly physical concrete tests needed, while also allowing the rapid analysis of a wide variety of "what if" type scenarios.

The main underlying program for the VCCTL (CEMHYD3D) has been described previously [1], as well as numerous applications based on using the underlying models [2, 3, 4, 5, 6, 7]. This User's Guide therefore provides a detailed description of the web-based user interface and a few examples of using the VCCTL to investigate specific problems of interest to the cement and concrete research community. This document is intended to be used as an online help utility: the VCCTL web forms are richly linked to the appropriate sections of this Guide.

DISCLAIMER

This software was developed at the National Institute of Standards and Technology by employees of the Federal Government in the course of their official duties. Pursuant to title 17 Section 105 of the United States Code this software is not subject to copyright protection and is in the public domain. The VCCTL is an experimental system. NIST assumes no responsibility whatsoever for its use by other parties, and makes no guarantees, expressed or implied, about its quality, reliability, or any other characteristic. We would appreciate acknowledgement if the software is used.

The U.S. Department of Commerce makes no warranty, expressed or implied, to users of the VCCTL and associated computer programs, and accepts no responsibility for its use. Users of the VCCTL assume sole responsibility under Federal law for determining the appropriateness of its use in any particular application; for any conclusions drawn from the results of its use; and for any actions taken or not taken as a result of analyses performed using these tools.

Users are warned that the VCCTL is intended for use only by those competent in the field of cement-based materials and is intended only to supplement the informed judgment of the qualified user. The software package contains computer models which may or may not have predictive value when applied to a specific set of factual circumstances. Lack of accurate predictions by the models could lead to erroneous conclusions with regard to materials selection and design. All results should be evaluated by an informed user.

INTENT AND USE

The algorithms, procedures, and computer programs described in this report constitute a prototype system for a virtual laboratory for the testing of cement and concrete. They have been compiled from the best knowledge and understanding currently available, but have important limitations that must be understood and considered by the user. The VCCTL system is intended for use by persons competent in the field of cement-based materials and with some familiarity with computers. It is intended as an aid in the materials selection, optimization, and design process.

2 Descriptions of Menu Selections

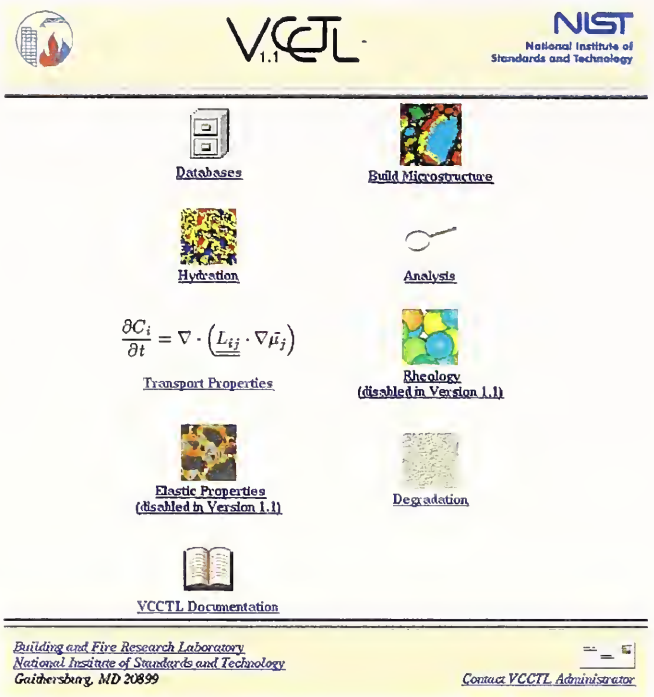


Figure 1: Main menu for the Virtual Cement and Concrete Testing Laboratory.

Upon entering the Virtual Cement and Concrete Testing Laboratory (VCCTL) system, the page shown in Figure 1 is displayed. The page consists of three frames. The top and bottom frames, which are tinted, are always displayed and contain links to common websites such as the National Institute of Standards and Technology (NIST) home page (upper right image), the Building and Fire Research Laboratory (BFRL) home page (upper left image), and the VCCTL main menu (upper middle image). The center frame (with white background) is the VCCTL Main Menu.

The main menu in earlier versions of VCCTL was composed of a list of descriptive actions. In Version 1.1, the main menu is subdivided into functional submenus, e.g.databases, build microstructure, hydration, etc., that reflect the order in which users commonly execute actions. Each of the submenus are discussed in the following subsections.

2.1 Databases submenu

Cement database For users of the VCCTL who do not have access to a scanning electron microscope (SEM) with X-ray imaging capabilities, a database of cement images has been created. With each installation of the software, a core set of fully characterized cements is stored in the database. Currently. this database contains 2-D images, quantitative image analysis results, and measured particle size distributions (PSDs) for 26 different cements produced in four different countries, as shown in Figure 2. The characterization process has been described in detail for two of the Cement and Concrete Reference Laboratory (CCRL) cements in a previously published report [6]. Typically, the PSD and quantitative phase analysis information will be used as input to construct a starting 3-D microstructure for a specific cement (see the **Build Microstructure submenu** section).

Upon entering the cement images database, the user will first be allowed to select a specific cement of interest using a fill-in form. Once this form is submitted, a 2-D color processed SEM/X-ray image will be returned along with the measured PSD for the chosen cement, as shown in Figure 3 for CCRL Cement 141, issued by the Cement and Concrete Reference Laboratory in June 2000. Below the image. the differential PSD (not shown in Figure 3) is tabulated on a particle diameter basis, in terms of both mass and number fractions. The number fractions have been obtained from the mass fractions based on the number of pixel elements present in digitized 3-D particles of each

Cement	Blaine (m^2/kg)	C_3S	C_2S	C_3A	C_4AF
CCRL Cement 135 (Jan. 2000)	394	0.6794	0.1714	0.0703	0.0789
CCRL Cement 136 (Jan. 2000)	390	0.6687	0.1848	0.0480	0.0985
CCRL Cement 140 (Jan. 2001)	402	0.6576	0.180	0.0994	0.0633
CCRL Cement 141 (June 2001)	397	0.6826	0.1147	0.1237	0.0790
U.S. Type I Cement	387	0.7038	0.1260	0.1170	0.0532
Turkish Cement	388	0.7012	0.1681	0.0651	0.0656

Note that phase fractions given above are on a volume basis!

Submit form for response

Figure 2: Portion of the form to select a cement from the cement images database.

specific diameter [1]. For small diameters (3 pixels and 5 pixels), it should be noted that the volume of the digitized sphere is significantly greater than that of a true sphere of equivalent diameter.

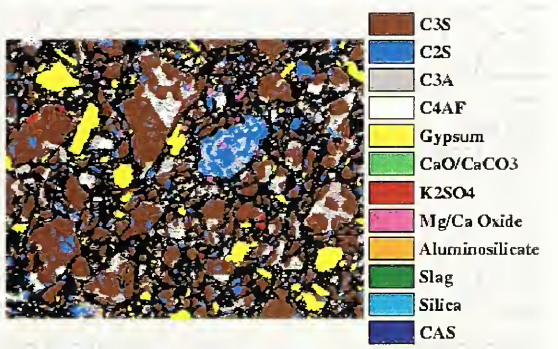


Figure 3: First half of page from cements image database for CCRL Cement 141, showing the new color scheme.

Figure 3 also indicates the new color coding scheme that has been adopted uniformly throughout VCCTL Version 1.1 software. The new colors mimic the approximate colors of the clinker phases when lightly etched with hydrofluoric acid and observed by reflected-light optical microscopy.

The page displayed for each cement also contains a link. About this cement, that directs the user to a second page containing the quantitative image analysis results for the cement, including the names of the computed correlation files which can be used to create "equivalent" 3-D microstructures.

2.2 Build Microstructure submenu

This submenu includes all of the functions required to create fully three-dimensional microstructures of cement paste that are ready for simulations of hydration. One of the unique aspects of the VCCTL models is the level of accuracy with which it constructs microstructures based on information from real cement powders. Aspects of microstructure that are faithfully reproduced by VCCTL software include the particle size distribution (PSD) of individual components, the volume fraction and surface area fraction of clinker compounds, volume fraction of mineral additions, and relative flocculation/dispersion of the cement paste.

2.2.1 Create a PSD file

This menu selection is used to create and store a particle size distribution (PSD) file which specifies the number of cement particles of each diameter to be placed in a starting 3-D microstructure. The

output file created by this selection can be specified as input to the next submenu item, **Generate initial microstructure**.

Entering the **Create a PSD file** submenu takes the user to a form shown in Figure 4, which requires the user to select a cement from the local database. Choosing any cement from the cement database will load information about the PSD of that cement, i.e., the mass fraction as a function of particle diameter. For each cement, these data are stored in the cement images directory, in a subdirectory for that cement name, in a text file having a `.psd` extension.

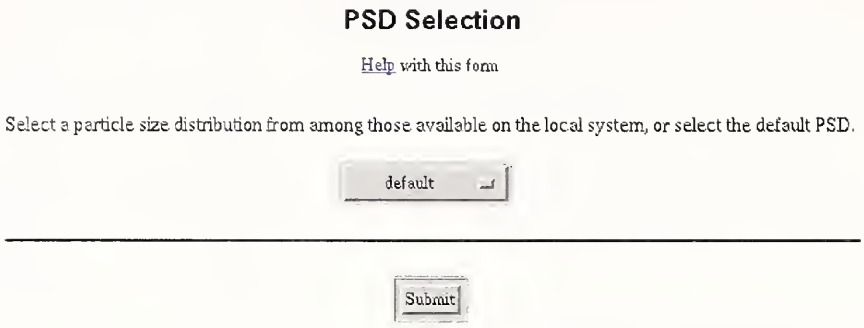


Figure 4: Form for selecting a cement PSD, system size, and system resolution.

Once the user submits this form, a second form is displayed. This form (shown in Figures 5 and 6) is used to actually specify PSD information, which will be written to a file. The components of the form are as follows:

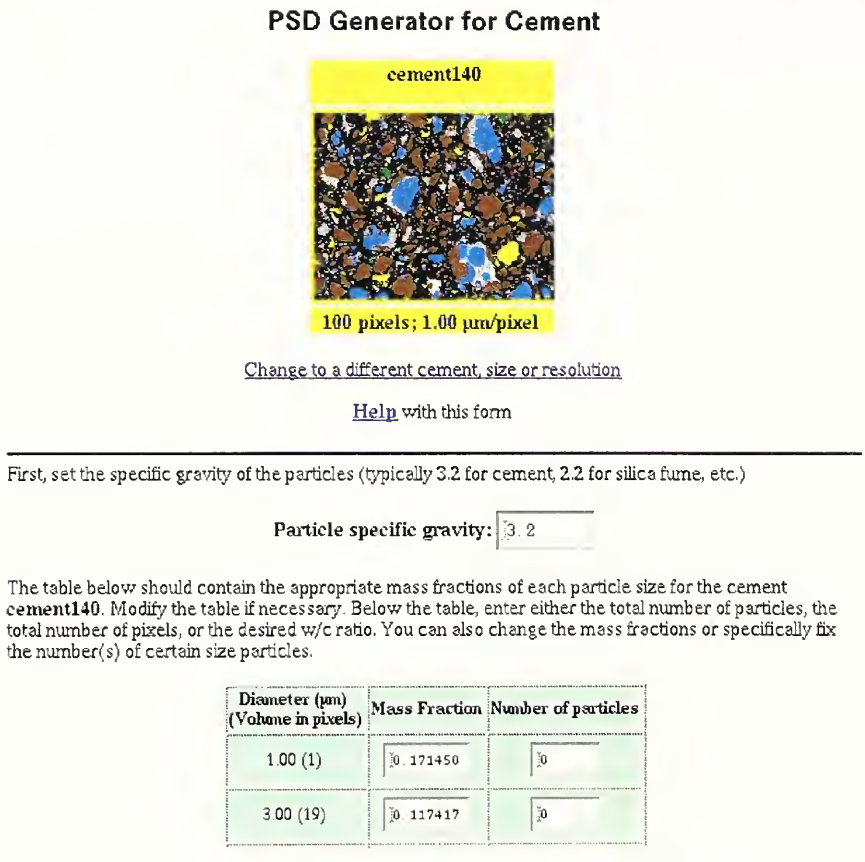


Figure 5: Top portion of the web form for creating a PSD file.

Selected cement To remind the user of the cement that was selected in the previous form, the name and an image of the cement is displayed at the top of the form, (see Figure 6), along with the chosen system size and resolution. A link is provided to return to the previous form if different settings are desired.

Particle specific gravity The user may specify the specific gravity of the particles in question. This form may be used to create particle size distribution files for many different compounds that will be present in a cement powder. Entering the specific gravity here allows the connection between mass fraction and volume that is required to calculate the number of particles to include in each size class. Common values for the specific gravity for different components are provided in Table 1.

Compound/Phase	Specific Gravity	Compound/Phase	Specific Gravity
Cement clinker	3.2	Fumed silica	2.2
Corundum	3.97	Quartz	2.64
Fly Ash	2.55	Gypsum (dihydrate)	2.32
Hemihydrate (bassanite)	2.73	Anhydrite	2.61

Table 1: Specific gravity of common cement phases and admixtures.

PSD Table This table lists the diameter, mass fraction, and number of particles for each size class. The mass fractions are taken directly from the cements database. The number of size classes (rows in the table) is determined by the values, entered on the previous form, for the system size and resolution. In particular, particle diameters (in pixels) that exceed 3/4 the system size are not allowed. Therefore, ordinarily they will not need to be edited, although they can be changed if the user desires. The user may enter the number of particles of each size class directly in this table, although this can be tedious and other methods are available (see below).

The final row of the PSD table contains the sums of each of the columns. The total mass fraction is present only to serve as a check that the sum of all the mass fractions is nearly unity; the value displayed in this field cannot be directly changed by the user, although a modification of one or more of the individual mass fractions will update its value.

The other entry in the final row of the table is the total number of particles. This value **can** be directly specified by entering a positive integer in the appropriate text field. The numbers of particles of each size class will automatically adjust, according to the mass fractions, to meet the specified total. In most circumstances, however, the total number of particles has little importance compared to the water-cement ratio or the total number of solid pixels, either of which may be specified as described below. If the user *does* wish to specify the total, the value entered must not be so large that more than 80 % of the system pixels are solids.

w/c ratio The user may request an approximate water-to-cement ratio here. Javascript code in the web page will automatically calculate the numbers of particles of each size class that most closely approximate that w/c. The number of particles and total number of pixels will also be updated. Note that the actual w/c ratio usually will not be equal to the value requested, because only whole numbers of particles of each size class are allowed. In particular, one too many large particles may result in a substantial decrease in the w/c. In this case, the user may manually set

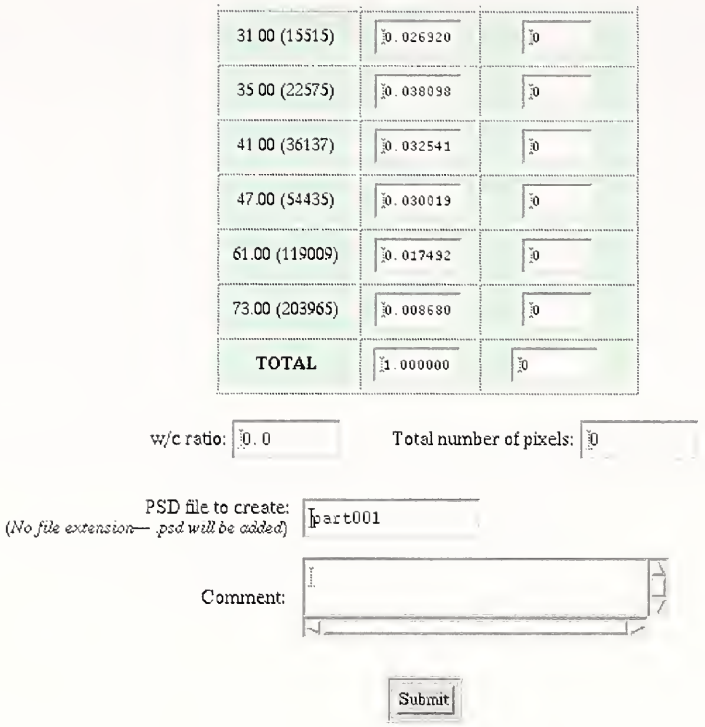


Figure 6: Bottom portion of the web form for creating a PSD file.

the mass fraction of these larger diameter particles to zero and repeat the automatic calculation by respecifying the desired value. Alternatively, if the intended simulations depend on the influence of coarse particles, or if the PSD of the cement is weighted heavily toward larger particles, then the user may manually decrease the numbers of smaller particles from several classes until the w/c ratio is closer to the desired value. This has limited impact if many large particles are required.

Total number of pixels The user may request an approximate total number of solid pixels (not particles), and the embedded Javascript code will automatically calculate the numbers of particles of each size that most closely approximate that total. Note that the actual pixel total usually will not equal the value requested, because only whole numbers of particles of each size class are allowed.

Specifying the total number of pixels often comes in handy when the user is attempting to construct a blended cement from several different materials (e.g., flyash, pozzolans, inert fillers etc). If the PSD file for the clinker already has been created by specifying w/c ratio, and if the total number of cement pixels is therefore known, then PSD files for a subsequent component can be made by calculating the number of pixels of that component needed to achieve the desired volume fraction of solid and using that value to create the new PSD. A step-by-step example of this procedure for creating a blended cement microstructure is provided in Appendix A.

Name of the particle file The data in the PSD table will be saved to a file for subsequent use in other calculations. Note that only the file root should be supplied (i.e., no file extension should be added) because the VCCTL software automatically appends the extension `.psd` to the name that is supplied. The file must have a unique name not already stored in the system; an error message

will be displayed otherwise.

NOTE: It is highly recommended that a notebook be used to keep a record of the filenames used, as well as any other pertinent information that may help the user remember the context under which the files were created. The output from the web forms, which contains all such relevant information, can be printed and stored in such a notebook if desired.

User comment The contents of this entry will be printed on the output page that is generated once the user submits this form. It exists to provide a reminder of the intent of the PSD file (e.g., what type of cement was selected, intended simulations, etc.)

Total mass fraction This field keeps a running sum of the mass fractions. In almost all cases, its value should be unity, which ensures a normalized PSD. Values significantly less than unity might indicate an error in the program or that the user has changed the mass fractions in the table.

Once the form is complete and the "Submit" button is clicked, an output page is generated. The output page contains all the vital information that was used to create the PSD file, along with the file name and any comments that the user entered. It is recommended that this output page be printed out because it contains the only record of the file name and any comments that the user included. The current version of VCCTL does *not* provide reminders of the available PSD file names later on.

2.2.2 Generate initial microstructure

This submenu is used to create an initial 3-D cement paste microstructure consisting of particles of cement, gypsum, and other selected compounds in water. The user may select the amount and form of gypsum, the particle size distribution, the presence or absence of flocculation in the paste, and the presence or absence of an aggregate particle in the system.

NOTE: The microstructure image created by this submenu is composed of single-phase particles only. For example, all cement particles are assigned to be C_3S (no C_2S, C_3A, or C_4AF is present), and any fly ash particles are supposed to be a non-descript "fly ash" phase. The distribution of phases among cement and fly ash particles is accomplished using the submenus named **Distribute cement phases** (Section 2.2.3) and **Distribute fly ash phases** (Section 2.2.6), respectively.

Entering this submenu leads to a page shown in Figure 7. The user is asked to select how the particle size distribution is to be specified. Under usual circumstances, the user already will have created a PSD file for this purpose. In this case, the button named "Read particle sizes from file(s)" should be selected. Otherwise, if the user wishes to manually type the numbers of particles of each possible size class, then the button named "Manual entry of particle sizes" should be selected. Either way, the only difference is that, if manual entry is selected, a long table is present for typing the numbers of particles of each size for each component, and for specifying the size and resolution of the system (see Section 2.2.1). Manual entry of particle sizes requires this table. If the user chooses to "Read particle sizes from file(s)", then the manual entry table will be absent and the form will be considerably shorter.

NOTE: It is **strongly** recommended that microstructures be created from previously-defined PSD

files rather than manual entry. Manual entry is tedious and prone to typographical errors that may go undetected.

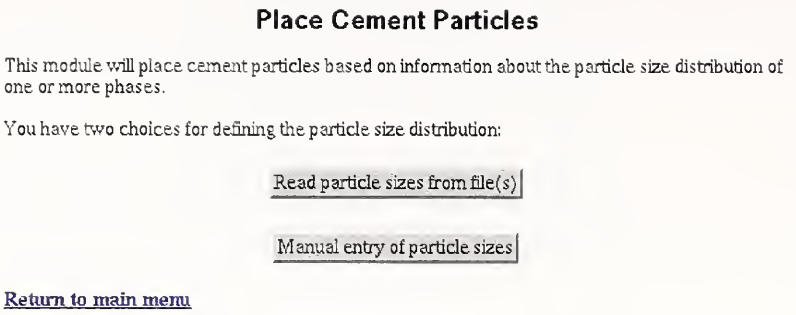


Figure 7: Entry page for creating an initial 3-D microstructure.

Read particle sizes from files(s) The form generated is shown in Figure 8 (top of the form) and Figure 10 (bottom of the form).

Random number seed The user must enter a *negative integer*, between -32767 and -1, in this field. The random number seed is used to initiate the sequence of the C random number generator that is used in the program. Random number seeds are requested in a number of web forms, such as those for generating the microstructure, distributing clinker phases, and hydration. Choosing the same random number seed for two different runs will guarantee the same sequence of random numbers that are produced during execution of the program.

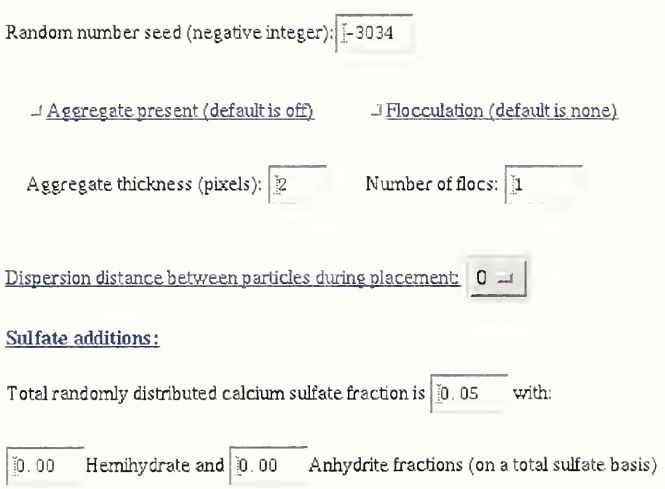


Figure 8: Top portion of the web form for creating an initial 3-D microstructure using pre-existing PSD files.

Aggregate present The user may choose to place a coarse aggregate particle in the 3-D microstructure. The aggregate particle is modeled as a flat plate of finite thickness. The flat-plate approximation is usually satisfactory for most applications because the surfaces of coarse aggregate particles typically have very low curvature compared to cement particles. Aggregate can be

included to study the formation of the interfacial transition zone (ITZ) microstructure as a function of cement PSD, mineral admixtures, hydration, etc. The default is to exclude aggregate from the 3-D microstructure. If selected, the user should also specify the aggregate thickness (an *even integer*) for the flat plate that will be centered in the 3-D microstructure. For further information and applications on the use of aggregate slabs in computer modeling of cements, see Refs. [8, 9, 10].

Flocculation The user may flocculate the cement particles after placing them in the 3-D microstructure. When a superplasticizer or high range water-reducing agent is not used, cement particles have a great tendency to flocculate together, perhaps into a single flocculated structure. Although this does not have a major effect on the long-term properties of hardened cement paste, it does significantly alter the rheological properties and setting behavior of the paste. When flocculation is enabled, the user must specify the numbers of flocs to be present after flocculation. For a totally flocculated system, this value would be 1, representing a single final floc (see Figure 9 for examples). The default behavior is to produce no intentional flocculation, although any given particle still might be placed at random in a position of incidental contact with one or more other particles. To ensure absence of any interparticle contacts, use the **Dispersion** option described in the next paragraph. For further information, consult Refs. [11, 12, 13].

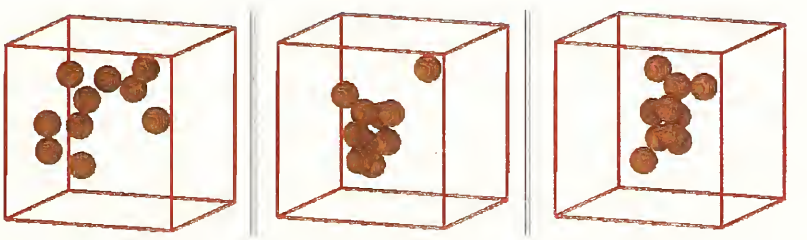


Figure 9: Varying degrees of flocculation among 10 equally sized cement particles. Left to right: no flocs, three flocs, and one floc.

Dispersion distance When a superplasticizer or high range water-reducing agent is used, the user may elect to disperse the cement particles to model the action of these specialty chemicals. A computational trick is used to place the particles with a radius either 1 or 2 pixels larger than their true radius. Since the placed particles cannot overlap, this will assure that all particles placed are at least 1 (or 2) pixels separated from all other particles. Note that for w/c ratios below about 0.4, this dispersion may not be possible due to the large number of particles typically present in the microstructure. In this case, the program genpartnew will issue an error message and exit without outputting the final microstructures to file. As with flocculation, dispersion does not significantly affect the long term properties of the hydrated cement paste, but can drastically alter the rheological properties and setting behaviors. For more information, see Refs. [11, 12, 13].

NOTE: The user should be aware that the physical distance between dispersed particles will also depend on the chosen resolution of the system, since the resolution determines the dimension of each pixel.

Sulfate additions The user has two options for placing calcium sulfate in the microstructure. If a separate PSD file for the sulfates is available, the user specifies that file later in the form. The form can even accommodate separate PSD files for the different *forms* of calcium sulfate: dihydrate,

hemihydrate, and anhydrite. However, if it is assumed that the calcium sulfate and cement have the same PSD, the user may just place particles as cement and choose to have a specific volume fraction of them randomly assigned as calcium sulfate afterward. In this case, the user must input the following in the form:

- the total volume fraction of solids that is some form of calcium sulfate
- the fraction *of the total calcium sulfate* that shall be **hemihydrate**
- the fraction *of the total calcium sulfate* that shall be **anhydrite**

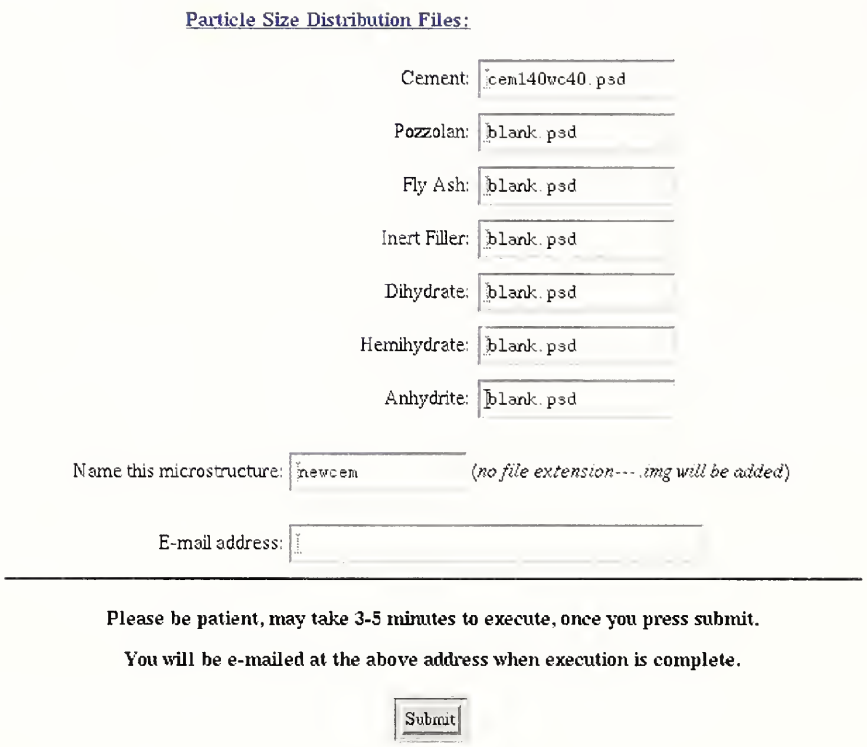


Figure 10: Bottom portion of the web form for creating an initial 3-D microstructure using pre-existing PSD files.

For example, suppose the system should have 0.02 volume fraction of dihydrate, 0.02 volume fraction of hemihydrate, and 0.01 volume fraction of anhydrite. Then the three numbers entered would be 0.05 (the sum of all three), 0.40, and 0.20, respectively. This will assign $0.05 \times 0.40 = 0.02$ volume fraction of the placed particles as hemihydrate and $0.05 \times 0.20 = 0.01$ volume fraction of the placed particles as anhydrite, randomly located throughout the microstructure, with the remainder (0.02) being distributed as the dihydrate form of calcium sulfate.

Particle size distribution files PSD files, created using the **Create a PSD file** submenu, may be specified for several phases/compounds as shown in Figure 10. The user should note that the PSD files themselves contain only the *number* of particles of each size class to add. If more than one PSD file is specified in the form, the numbers for each size class in each file are summed. The user bears the responsibility of ensuring that the PSD files were all created in such a way as to produce the desired water-to-solids ratio.

Any of the compounds listed in Figure 10 that do *not* have an associated PSD file must have "blank.psd" entered in their field(s). For this reason, this is the default name that appears in each entry except that for cement.

Only particles ≥ 3 pixels in diameter are added during the particle placement routine. All one-pixel particles must be added during the specification of the hydration itself. This is done to allow the optional flocculation of the 3-pixel-diameter and larger particles during the creation of the 3-D particle microstructure image. Because the 1-pixel particles are generally quite large in number, their inclusion in the flocculation algorithm would result in dramatic increases in the memory and time requirements of the 3-D microstructure creation program.

Name this microstructure The information in this web form will be used to create a microstructure "image" file that can be used in subsequent calculations or simulations. Note that only the file root should be supplied (i.e., no file extension should be added) because the VCCTL software automatically appends the extension `.img` to the name that is supplied.

Particle image file When a 3-D microstructure is initially generated, *two* image files are actually created: (1) the microstructure image file itself, in which each pixel carries an integer label that specifies its phase and (2) a **particle** image file, in which each pixel carries an integer label that specifies the particle to which each pixel belongs (these latter labels range from 1 to the number of particles in the image). The particle image file is used in subsequent calculations to determine percolation properties during hydration [1] and, in some cases, to distribute fly ash phases on a particle basis (see Section 2.2.6). The name for the particle image file is automatically generated (no user input required) by placing the character "p" at the beginning of the microstructure image file specified in the form.

E-mail address Some of the calculations performed by VCCTL may take several minutes to complete. The user may enter an e-mail address to which a note will be automatically sent upon completion of the calculation. If no e-mail address is supplied, then a note will not be generated.

Again, once the user verifies that all the information on the form is correct and presses the "Submit" button, an output page is generated with all the relevant information, including the name of the microstructure image file. It is recommended that the output page be printed and kept as a record of the file name that was chosen.

2.2.3 Distribute cement phases

Once an initial arrangement of generic cement (and gypsum, fly ash, etc.) particles in water has been created, the user may use this submenu to distribute the four major cement clinker phases—C_3S, C_2S, C_3A, and C_4AF—amongst the cement particles. To do this, the 3-D microstructure image is filtered using two-point correlation functions measured on the actual 2-D SEM images of any processed cement in the cements database [1, 2, 6]. The filtering process, subsequent thresholding, and adjustments to the average mean curvature of the interfaces, are conducted in such a way as to match the volume and surface area fractions previously determined for each of the four major cement clinker phases.

Clicking the **Distribute cement phases** link leads to the page shown in Figure 11, which requests two items:

Name of original microstructure file This must be the name of a 3-D microstructure image (extension `.img`) that has not had the cement phases distributed already, i.e., any microstructure image that was not created previously using this form. Typically, this will be a file created previously by using the **Generate initial microstructure** submenu (Section 2.2.2).

Match distribution data using cement: This is the name of the characterized cement that will be used to match the two-point correlation functions. All of the cements recorded in the cements database (see Section 2.1) should be available for selection.

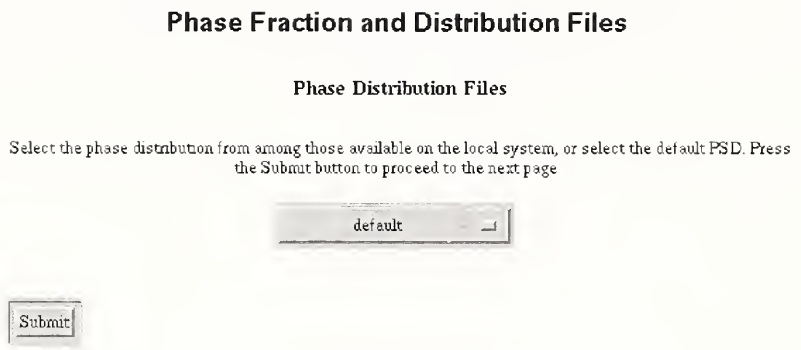


Figure 11: Entry page for distributing cement phases amongst cement particles in a 3-D microstructure image.

Upon pressing the "Submit" button on this page, a second form is displayed, as shown in Figure 12 (the topmost portion of this form, which displays an image of the cement selected, is omitted from the figure). A description of the form entries is provided below.

Version 1.0 file detected This message appears only if the name of the original microstructure file, entered in the previous form, appears *not* to have been created using VCCTL Version 1.1. In this case, Version 1.1 does not have access to several items of information, such as the particle image file, the number of one-pixel particles, etc. used during creation of the original file.

When a Version 1.0 file is detected here, the user is prompted for the name of the **particle** image file that was generated during creation of the original file. Unless the user has intentionally changed the naming convention in some way, the particle image file will have the same name as the original microstructure file, entered on the previous form, except that the character "p" is added at the beginning. This is the default name provided in this field. With a valid particle image file name, and an automatic scan of the original microstructure file, the software should be able to convert the file to Version 1.1 format.

NOTE: Version 1.1 *cannot* determine the numbers and types of one-pixel particles that should be added to microstructure that was created using Version 1.0. Therefore, when submitting a request for hydration of such a microstructure, the user will need to calculate the numbers and types of one-pixel particles using the online worksheet that is accessible from the hydration form (see Section 2.3.4 for a description).

Random number seed The user must enter a *negative integer* (in the range [-32767,-1]) in this field. See the description in Section 2.2.2 for more information on the purpose of random number seeds in VCCTL.

Filename of original microstructure This must be the name of a 3-D microstructure image (extension `.img`) that has not had the cement phases distributed already, i.e., any microstructure image that was not created previously using this form.

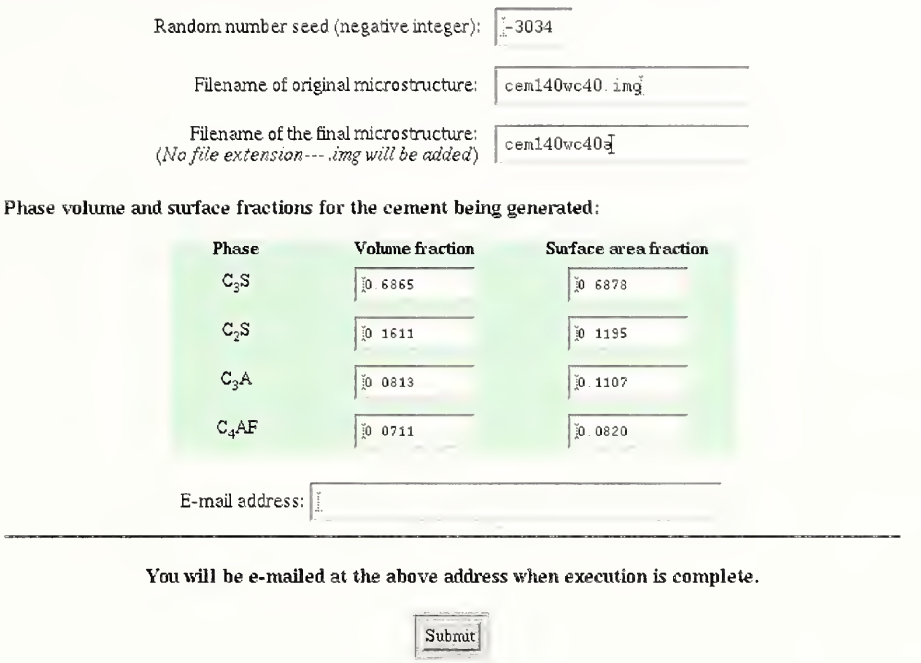


Figure 12: Form for distributing cement phases amongst cement particles in a 3-D microstructure image.

Filename of the final microstructure Enter the name that you wish the processed microstructure to have after the four major cement clinker phases have been processed. As in previous forms already described, only the file root name should be supplied here; the extension `.img` will be added automatically.

Phase volume and surface fractions The default values shown in these fields are the volume fractions and surface fractions of each phase already calculated for the cement that was selected on the previous form. These data are taken directly from the cements database. Therefore, under ordinary circumstances they will require no adjustment. The user is free to change the values that are shown. However, caution must be exercised to ensure that the values of each column sum to 1.0.

E-mail address Using current single-processor hardware, the program `distrib3d` that performs the distribution of cement phases requires a minimum of 20 min. The actual time to completion depends on the speed of the processor as well as the CPU load. The VCCTL will automatically send a note to the e-mail address provided when execution completes. If no e-mail address is supplied, then a note will not be generated.

NOTE: After the distributed microstructure image has been created, it is a good practice to check immediately that the target volume fractions and surface fractions of the clinker phases have been achieved with satisfactory accuracy. This can be done using the **Phase statistics** submenu of the **Analysis menu** (see Section 2.4.1 for details). Any problems can be corrected at this point before proceeding with lengthy simulations of hydration.

NOTE: The VCCTL is set up to perform up to two concurrent phase distributions. If a phase distribution request is submitted while two others are being executed, the user will be notified to resubmit the request at a later time.

2.2.4 Filter to distribute only two cement phases

Normally, the user will use the submenu entry described in Section 2.2.3 (**Distribute cement phases**) to automatically distribute all four phases amongst the initial cement particles. However, for those experiments in which special control over the distribution process is needed, the user may execute each step in the distribution process separately. For any specified cement, these steps involve repeated application of the following three actions:

1. Filter a 3-D image using a specified two-point correlation function for a specified cement (described here)
2. Check the phase volume and surface statistics (described in Section 2.4.1)
3. Adjust the hydraulic radius of a single phase (described in Section 2.2.5)

This submenu entry accomplishes the first of these actions. Basically, an image of random noise is superposed on the random particle microstructure image and filtered by (convolved with) the correlation function for one or more phases determined from the 2-D SEM images. Then, the correlated noise image is thresholded to separate one phase of the microstructure into two phases, with the user specifying the desired volume fraction of each phase. For example, initially, the cement particles are separated into silicates and aluminates using a `cemXXX.sil` correlation function file [1]. In subsequent passes of this algorithm, the silicates are separated into C_3S and C_2S, while the aluminates are separated into C_3A and C_4AF.

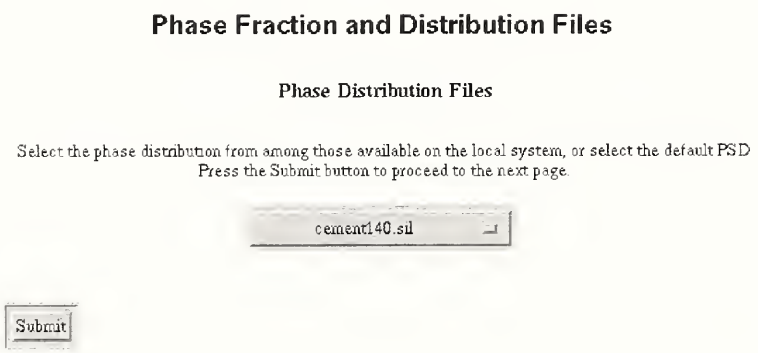


Figure 13: Entry page for distributing cement phases amongst cement particles in a 3-D microstructure image.

Upon selecting this submenu entry, the page in Figure 13 is displayed, in which the user is asked to choose the specific two-point correlation file, from among those in the cements database, that will be used for the calculation. The choices have names of the form `fileroot.xxx`, where

- `fileroot` is the name of the cement used in the cements database
- `xxx` specifies the phases used to create the two-point correlation function file:
  - `sil`: silicates (C_3S and C_2S) are separated from aluminates (C_3A and C_4AF)
  - `c3s`: C_3S is separated from C_2S (this is used after the silicates have been separated from aluminates)
  - `c3a`: C_3A is separated from C_4AF in cements for which the volume fraction of C_3A is greater than that of C_4AF (this is used after the silicates have been separated from aluminates)
  - `c4a`: C_4AF is separated from C_3A in cements for which the volume fraction of C_4AF is greater than that of C_3A (this is used afte the silicates have been separated from aluminates)

Once the user selects a correlation function file and presses the "Submit" button. a second page is displayed as shown in Figure 14 (the top portion of this form, which displays an image of the cement, is omitted from the figure). The entries in this form are described below.

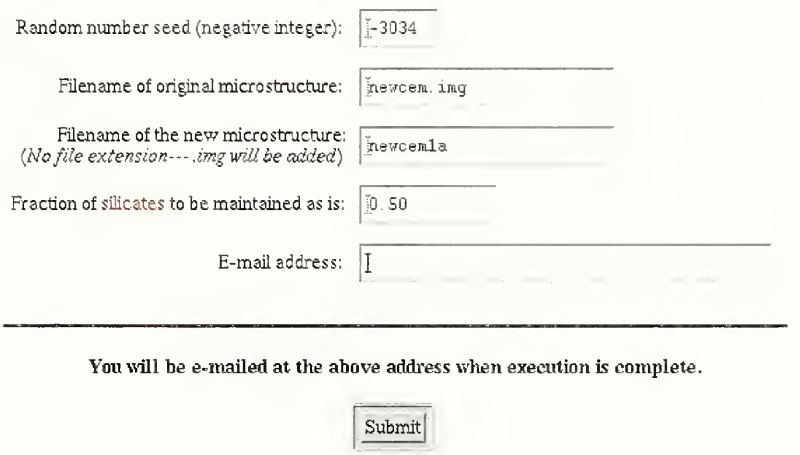


Figure 14: Form for distributing two cement phases in a 3-D microstructure image.

Random number seed The user must enter a *negative integer* (in the range [-32767,-1]) in this field. See the description in Section 2.2.2 for more information on the purpose of random number seeds in VCCTL.

Filename of original microstructure This must be the name of a 3-D microstructure image (extension `.img`) that has not had the cement phases distributed already. i.e.. any microstructure image that was not created previously using this form.

Filename of the new microstructure Enter the name that you wish the processed microstructure to have after this phase separation has been accomplished. As in previous forms already described, only the file root name should be supplied here: the extension `.img` will be added automatically.

Fraction of *xxx* to be maintained as is Here, *xxx* can be "silicates", "C_3S", "C_3A", or "C_4AF", depending on the file selected in the previous form.

E-mail address The program `rand3d` that performs the distribution of cement phases takes less time to execute than does the program `distrib3d` described in the previous section, but the wait can still be significant. The VCCTL interface automatically sends a note to the e-mail address provided when execution completes. If no e-mail address is supplied, then a note will not be generated.

NOTE: The VCCTL is set up to perform only one of these types of phase distributions at a time. Therefore, if the system is busy with one request when another request is submitted, the user will be notified to resubmit the second request at a later time.

2.2.5 Adjust the hydraulic radius of one phase

Following the filtering process (see Section 2.2.4), the surface area fractions of the filtered phases—which can be checked as described in Section 2.4.1— may not match those of the phases in the starting 2-D SEM images. These surface area fractions can be adjusted using a 3-D "sintering" algorithm to swap specific locations of the two phases in a manner that obtains the desired surface area fractions. Details of the 3-D sintering algorithm have been published previously [14, 15], with the specific application to cement particles described in the CEMHYD3D Version 2.0 User's Manual [1].

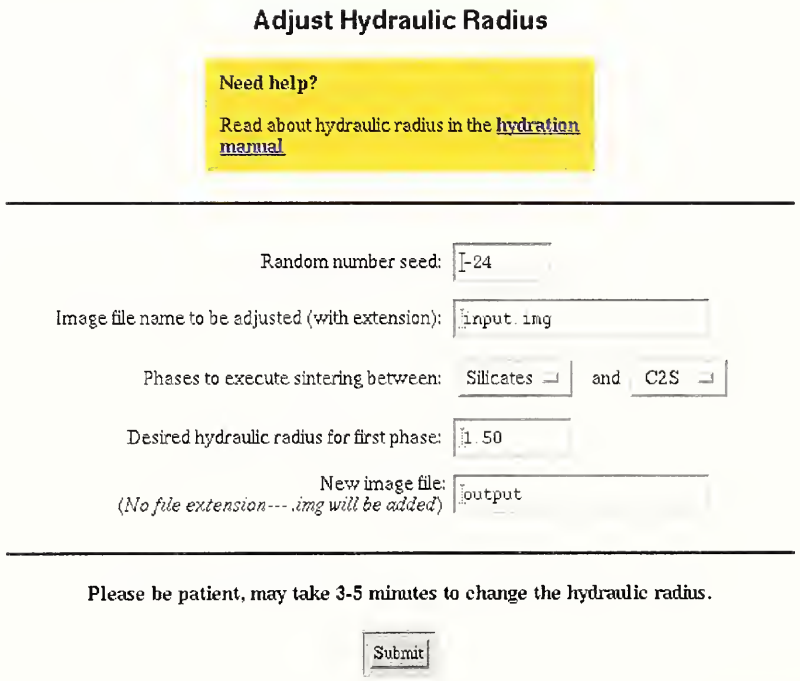


Figure 15: Form for adjusting the hydraulic radius of the surfaces of a single phase in a 3-D microstructure image.

The input form, shown in Figure 15, has the following entries:

Random number seed The user must enter a *negative integer* (in the range [-32767.-1]) in this field. See the description in Section 2.2.2 for more information on the purpose of random number seeds in VCCTL.

Image file name to be adjusted This must be the name of any 3-D microstructure image (extension `.img`) that contains at least the two phases defining the interface that is to be modified by this action.

Phases to execute sintering between The algorithm increases the hydraulic radius of the first phase by selecting n pixels of that phase that have the n highest values of mean curvature—using capillary porosity to determine the surface—and switching the identity of those pixels to that of a second phase. To conserve volume of each phase during the process, n pixels of the second phase having the n lowest values of mean curvature—using either capillary porosity **or** the second phase itself to determine the surface—have their identity switched to that of the first phase [14].

Desired hydraulic radius for first phase If one already knows the desired surface area (in number of pixels) of the first phase, then the desired hydraulic radius R_h can be calculated using the following equation:

$$R_h = \frac{3V}{2S} \tag{1}$$

where V is the volume (in number of pixels) of the first phase. V for any phase can be found by computing the phase statistics as described Section 2.4.1. The factor 3/2 is included to correct for the difference between the approximate surface area of a digitized (pixel-based) sphere and a continuum sphere of the same diameter.

NOTE: The hydraulic radius of a phase can only be *increased* when applying the sintering algorithm to it. If it is necessary to decrease the hydraulic radius of a phase, the algorithm should be executed so as to increase the hydraulic radius of the secondary phase, thus decreasing that of the primary one [1].

New image file Enter the name that you wish the processed microstructure to have after this phase separation has been accomplished. As in previous forms already described, only the file root name should be supplied here; the extension `.img` will be added automatically.

E-mail address The program `sinter3d` that performs the adjustment to the hydraulic radius may take several minutes to complete. The VCCTL interface automatically sends a note to the e-mail address provided when execution completes. If no e-mail address is supplied, then a note will not be generated.

2.2.6 Distribute fly ash phases

The user may create initial 3-D microstructures with a number of "generic" fly ash particles (see Section 2.2.2 for details). The distribution of phases comprising fly ash particles may be accomplished within those generic fly ash particles, under one of two simplifying cases, by using this

submenu. The form that appears is shown in Figure 16 (top of the form) and Figure 17 (bottom of the form).

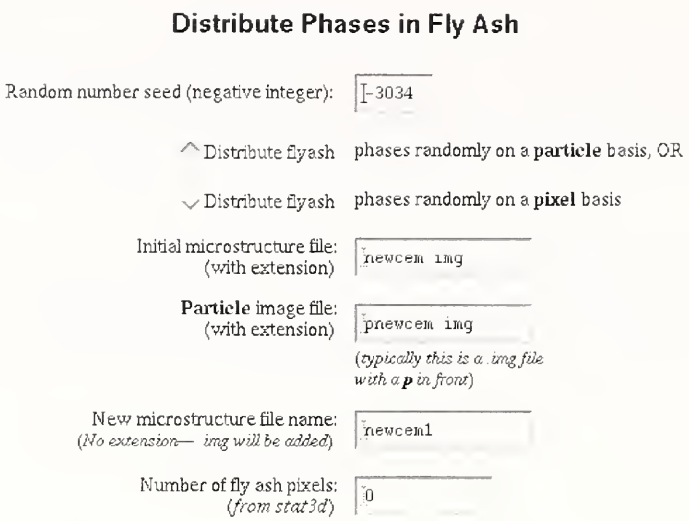


Figure 16: Top portion of the form for distributing fly ash phases within "generic" fly ash particles.

Random number seed The user must enter a *negative integer* (in the range [-32767,-1]) in this field. See the description in Section 2.2.2 for more information on the purpose of random number seeds in VCCTL.

Method for distributing fly ash phases The user has two choices:

1. **Particle basis**. Each particle is assumed to be comprised of a single phase, and the **particles** are randomly assigned phases to achieve a close approximation to the desired phase volume fractions specified in the table at the bottom of the form (see Figure 17). The program that executes this method is called `distfapart`.

2. **Pixel basis**. The phases are simply randomly distributed amongst all the generic fly ash *pixels* to achieve the volume fractions specified in the table at the bottom of the form (see Figure 17). This method produces a very fine and relatively uniform distribution of the fly ash phases within the individual particles. The program that executes this method is called `distfarand`.

Initial microstructure file This must be the name of any 3-D microstructure image (extension `.img`) that contains generic fly ash particles.

Particle image file This must be the name of the particle image file associated with the microstructure file already specified in the previous entry. For more information on the particle image file, see Section 2.2.2. Because the same particle image file may be associated with any number of microstructure image files, this file name is requested separately instead of being automatically constructed from the name of the microstructure image file.

New microstructure file name Enter the name that you wish the processed microstructure to have after this phase separation has been accomplished. As in previous forms already described, only the file root name should be supplied here; the extension `.img` will be added automatically.

Number of fly ash pixels This number can be determined by computing the spatial statistics of the microstructure image, as described in Section 2.4.1.

Phase fractions Currently, the following phases are considered for distribution amongst the fly ash particles: aluminosilicate, calcium aluminodisilicate, silica, anhydrite, calcium chloride, tricalcium aluminate, and an inert phase. Reactions between these phases and the main components of cement have been incorporated into the current version of the cement hydration model [1, 16]. A warning message will appear if the user attempts to specify phase fractions the sum of which exceeds 1.0.

E-mail address On most computers, either program `distfarand` or `distfapart` will execute within one minute. Nevertheless, the user has the option to specify an e-mail address to which an automatically-generated note will be sent upon completion of the calculation.

Figure 17: Bottom portion of the form for distributing fly ash phases within "generic" fly ash particles.

2.3 Hydration submenu

This submenu provides access to the NIST 3-D cement hydration model. In addition, it also provides utilities for creating a curing temperature schedule file, which is required by the hydration model under certain conditions.

2.3.1 Specify a temperature schedule (curing)

The CEMHYD3D cement hydration model can be executed under one of three thermal conditions: isothermal, adiabatic, or user-programmed temperature schedule. This menu selection is used to specify a controlled temperature schedule to be used throughout the hydration process. Clicking on the submenu entry generates a form shown in Figure 18. If the user is planning to cure under isothermal or adiabatic conditions only, then this step can be skipped.

Temperature schedule file name A name either of a new file or an existing temperature schedule file, to which additional data are to be appended, should be entered here.

Status of file The user may indicate whether the file is (1) created as a new file or (2) opened as an existing file for appending the new data. In previous versions of VCCTL, the user was limited to six separate temperature ramps or dwell periods. In Version 1.1 the user may append new data to an existing file, which effectively removes all constraints on the number of separate entries in a temperature schedule.

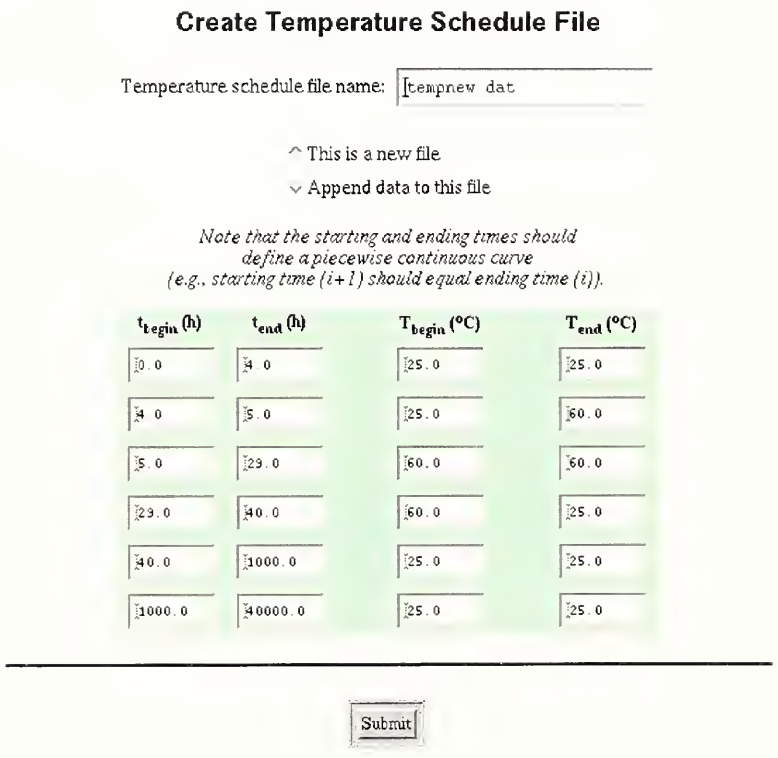


Figure 18: Form for specifying a programmed temperature schedule for controlled curing.

Data table The user may specify up to six separate temperature ramps or dwell periods in the table. Each ramp or dwell period is represented by a linear segment in a piecewise-continuous function of temperature versus time. The user simply indicates the starting and ending times and the starting and ending temperatures for each segment, which uniquely specifies the slope of that segment (dwell periods have the same starting and ending temperatures. and so by definition have zero slope). For any segment i, the ending time $t_{i,\mathrm{f}}$ is forced to equal the beginning time, $t_{i+1,0}$. of segment $i+1$.

2.3.2 Specify slag characteristics

This feature is currently under development within the Virtual Cement and Concrete Testing Laboratory.

2.3.3 Specify alkali characteristics

This feature is currently under development within the Virtual Cement and Concrete Testing Laboratory Consortium.

2.3.4 Hydrate a 3-D microstructure

The NIST cement hydration model operates directly on 3-D images of cement paste microstructure. such as those commonly generated using VCCTL software under the **Build Microstructure** submenu. Execution of the hydration model requires a starting microstructure. information about the curing conditions, knowledge of the availability or absence of excess water, and specifications of the frequency with which properties will be calculated and written to data files during the course of hydration. Clicking on this submenu entry generates a sequence of web forms. the first of which is shown in Figure 19, that guide the user in specifying all of this information so that a simulation of hydration can be properly launched.

Step 1: Starting microstructure

This form contains only two fields, as shown in Figure 19:

Random number seed The user must enter a *negative integer* (in the range [-32767,-1]) in this field. See the description in Section 2.2.2 for more information on the purpose of random number seeds in VCCTL.

Name of initial microstructure This should be the name of a valid microstructure image file (extension `.img`) and commonly will be one that has already had the four major clinker phases distributed (see Section 2.2.3 for more information). The web interface programs use this information, not only to supply the model with the file name. but also to construct the name of the corresponding *particle* image file (see Section 2.2.2) and the `.info` file that contains information on

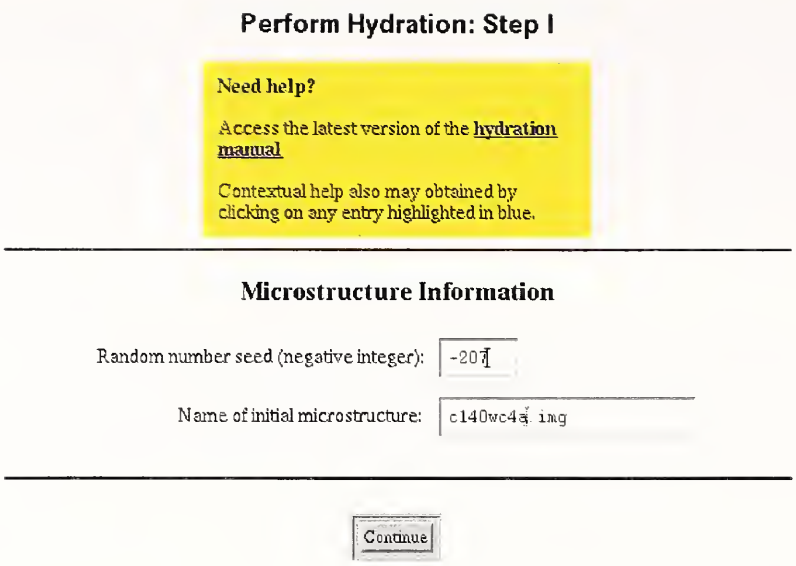


Figure 19: First of five forms for launching the VCCTL hydration model.

the phase fractions and calculated numbers of one-pixel particles from the particle size distribution (PSD).

Step 2: Other microstructure information

This form, shown in Figures 20 and 22, appears after submitting the previous form by pressing its "Continue" button. It collects information about the number of one-pixel particles to place in the microstructure prior to hydration, and also about the volume fraction of aggregate if one is simulating hydration of the cement paste within concrete.

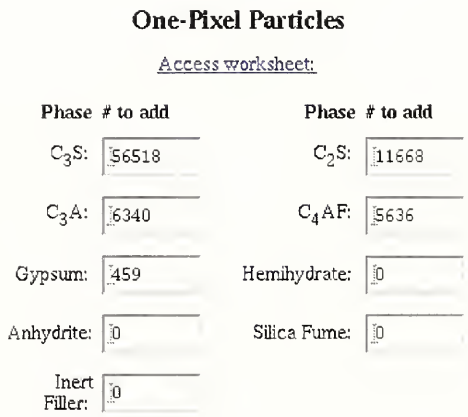


Figure 20: Top portion of the second of five forms for launching the VCCTL hydration model.

Version 1.0 file detected This message appears only if the name of the original microstructure file, entered in the previous form, appears *not* to have been created using VCCTL Version 1.1. In this case, Version 1.1 does not have access to several items of information, such as the particle image file, the number of one-pixel particles, etc. used during creation of the original file.

When a Version 1.0 file is detected here, the user is prompted for the name of the **particle**

image file that was generated during creation of the original file. Unless the user has intentionally changed the naming convention in some way, the particle image file will have the same name as the original microstructure file, entered on the previous form, except that the character "p" is added at the beginning. This is the default name provided in this field. With a valid particle image file name, and an automatic scan of the original microstructure file, the software should be able to convert the file to Version 1.1 format.

NOTE: Version 1.1 *cannot* determine the numbers and types of one-pixel particles that should be added to microstructure that was created using Version 1.0. Therefore, when submitting a request for hydration of such a microstructure, the user will need to calculate the numbers and types of one-pixel particles using the online worksheet that is accessible from the hydration form (see below for description).

One-pixel particles In previous versions of VCCTL, the determination of the correct number of one-pixel particles involved tedious calculation based on the individual PSDs and volume fractions of the anhydrous phases. In Version 1.1, however, much of this information is "remembered" and automatically uploaded to the form if the microstructure was created in the usual way described earlier in this User's Guide. Therefore, under normal circumstances, the user will not need to adjust the values that are displayed on the form. Of course, the user is free to change the values at his/her discretion.

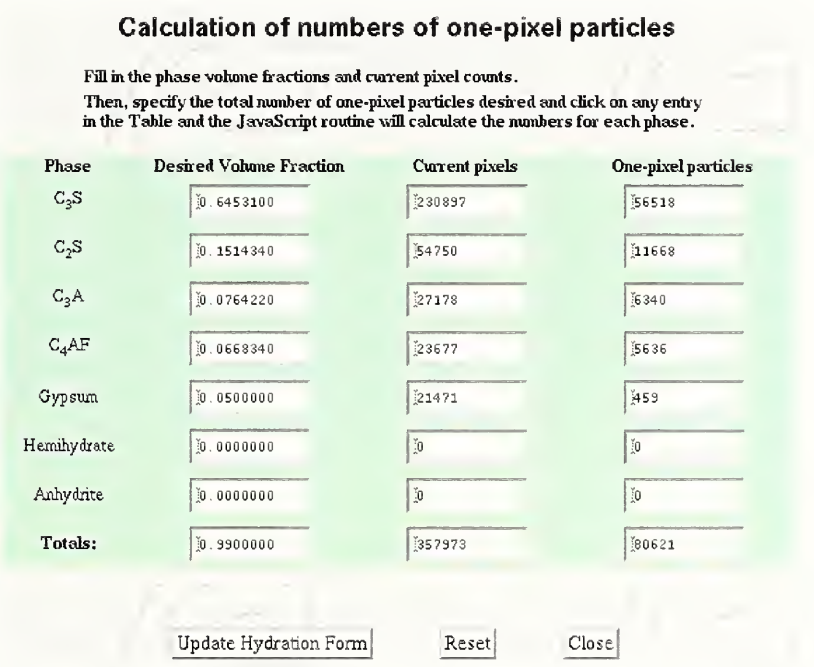


Figure 21: Supplemental worksheet for calculating the numbers of one-pixel particles of each major cement phase to be placed prior to hydration.

If the starting microstructure was created using any VCCTL version prior to 1.1, then the user must calculate the numbers of one-pixel particles. As an aid in this calculation, a worksheet is provided (see Figure 21). The worksheet will calculate the number of one-pixel particles of each of the four major clinker phases, as well as the various forms of calcium sulfate, based on the current number of pixels and targeted volume fractions of each of these phases in the microstructure. The current number of pixels of each phase may be obtained as described in Section 2.4.1. This form

was also available in Version 1.0, but in Version 1.1 it has the additional feature that the data can be transferred directly from the completed worksheet to the form by pressing the "Update" button on the worksheet.

Other one-pixel particles One-pixel particles of any phase recognized by the hydration model can be added to the microstructure prior to hydration. To add them, the user simply enters the phase identification for the desired phase and the number of one-pixel particles of that phase that are desired (see Figure 22). If the phase identification number of a particular compound is not known, clicking on the Phase ID link will display the list of all available phases and their corresponding integer identification numbers. Up to two additional phases can be specified in this way.

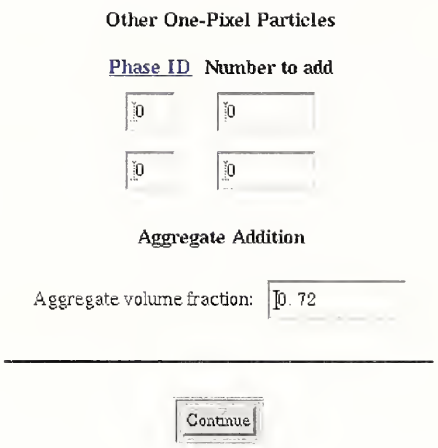


Figure 22: Bottom portion of the second of five forms for launching the VCCTL hydration model.

Step 3: Curing and kinetics

This is the third form in the sequence of five, and appears upon clicking the "Continue" button at the bottom of the previous form. The top portion of the form is shown in Figure 23. This form collects information about the time of hydration, specifications about the thermal conditions and availability of excess water, and data on the average apparent activation energies of the major hydration reactions.

Number of hydration cycles The hydration model operates by a sequence of steps: dissolution (in which solid pixels may detach from the solid to become mobile agents in the pore solution), random-walker diffusion of the mobile agents, and (possible) reaction between colliding pixels. One complete sequence of these steps is called a *cycle*. Although cement pastes of different composition and w/c ratio will produce different results, a typical Type I ordinary Portland cement with w/c = 0.40 will often set at ≈100 cycles (the default value on the form), and the capillary pore space will become disconnected at ≈500 cycles. Furthermore, Figure 24 shows the relationship between degree of hydration, α, and number of cycles for CCRL Cement 140 with w/c = 0.40.

Terminate when degree of hydration reaches ... This entry is optional. If the user would like the hydration to terminate as soon as a particular value of the degree of hydration (mass basis) has been achieved, that value may be entered here. The simulation will terminate when either this

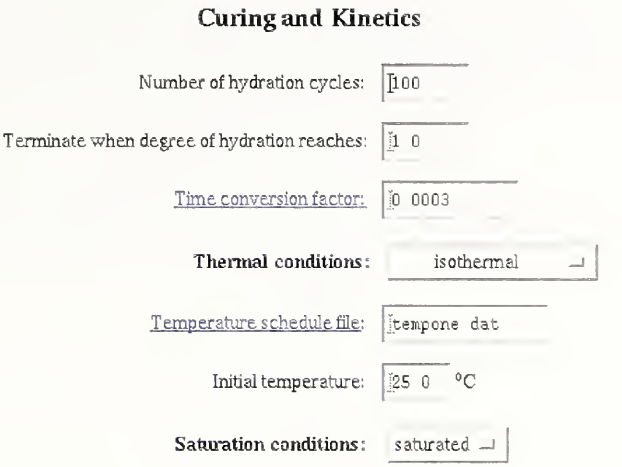


Figure 23: Top portion of the third of five forms for launching the VCCTL hydration model.

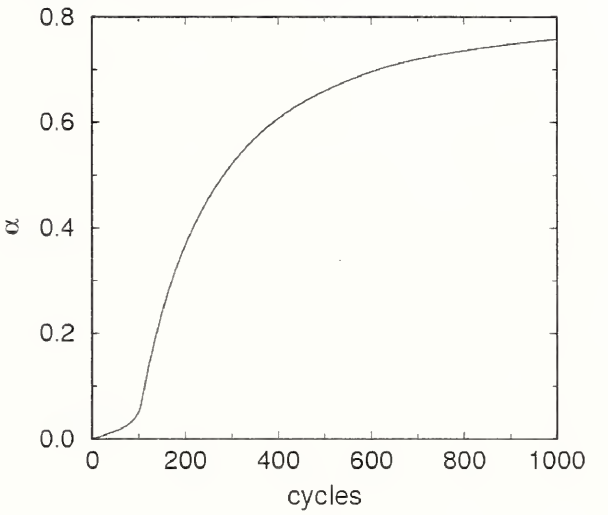


Figure 24: Plot of degree of hydration (α) versus number of hydration cycles for CCRL Cement 140 having w/c = 0.40. Curing was simulated at 25 °C under saturated conditions.

degree of hydration has been achieved, *or* when the specified number of hydration cycles has been executed. whichever happens first. By specifying 1.0 (the default value on the form) the simulation will execute for the number of cycles specified in the previous entry.

Time conversion factor Hydration cycles have no intrinsic time scale. In the current version of VCCTL, hydration time t is related to the number of cycles n by the empirical relation

$$t = \beta n^2 \tag{2}$$

where β is the *time conversion factor* that is requested in this form entry. β has units of reciprocal time, and typical values for β are ≈ 0.0003 h^{-1} (the default value on the form) for a normal Type I Portland cement, and ≈ 0.0005 h^{-1} for a low-alkali cement.

It should be noted that the transformation in Eq. (2) is employed not for any fundamental reason, but rather because it often provides a reasonable fit to experimental measurements of α vs.

t. A loose physical justification of the parabolic form of Eq. (2) is that diffusion through semipermeable hydration product, which obeys parabolic kinetics, becomes increasingly rate-controlling as hydration proceeds.

Thermal conditions The next several form entries relate to the thermal conditions employed throughout curing. The first one involves choosing the thermal boundary conditions on the system, and the options are

1. **Isothermal**, for which it is assumed that the system is in diathermal contact with a constant-temperature reservoir and that heat transfer is sufficiently rapid to ensure that the system maintains the same constant temperature as the reservoir.
2. **Adiabatic**, for which it is assumed that the system is thermally isolated from its surroundings.
3. **Temperature-defined**, for which a pre-programmed temperature schedule is assumed to control the temperature of the system. See Section 2.3.1 for information on creating a temperature schedule for use with this option.

Temperature schedule file A valid temperature schedule file must be entered in this field *only* if the user chooses to use "temperature-defined" thermal conditions in the previous selection. Under isothermal or adiabatic/semi-adiabatic conditions, this field will not be used whether or not it contains a valid file name.

Initial temperature The initial temperature is the starting temperature of the cement paste system. If hydration is being executed under a controlled temperature schedule, then the initial temperature of the temperature schedule overrides any value entered in this field.

Saturation conditions The user has two options from which to choose:

1. **saturated**, for which the cement paste is assumed to be in contact with a reservoir of excess water. As free water in the capillary pore space is consumed by the hydration process, it is immediately replaced by water from the reservoir. Note, however, that once the capillary porosity reaches its percolation threshold and becomes disconnected, water replacement is no longer possible.
2. **sealed**, for which free water consumed during hydration is not replaced. Instead, the capillary pore space is progressively emptied of its water, starting in those pore regions with the largest effective diameters.

The bottom portion of the third form is shown in Figure 25. The form fields in this portion of the form relate to apparent activation energies of the main reactions that occur during hydration.

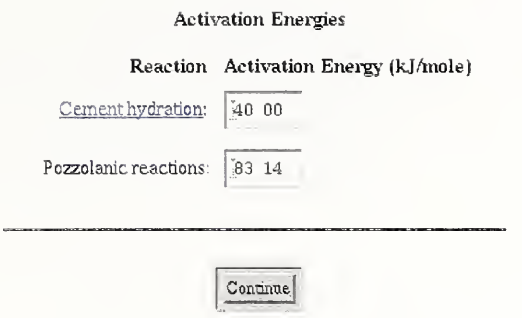


Figure 25: Bottom portion of the third of five forms for launching the VCCTL hydration model.

Cement hydration For the present purposes, the process of cement hydration is considered as a single composite reaction with a characteristic apparent activation energy which could be measured in principle by making an Arrhenius plot of the rate of consumption of anhydrous phases vs. $1/T$. For a Type I cement, if no further information is available, ASTM C 1074 [17] suggests a value of 40 kJ/mol.

Pozzolanic reactions The dissolution of portlandite (CH) due to pozzolanic influence is assumed to be a thermally activated process, and the activation energy entered here is used to calculate the intrinsic rate of dissolution as a function of temperature according to an Arrhenius expression of the form

$$k = k_0 \exp\left(\frac{-E_a}{RT}\right) \tag{3}$$

where k_0 is the reaction rate constant extrapolated to temperature $T = 0$, E_a is the activation energy requested here, in units of kJ/mol, and R is the gas constant in units of kJ/(mol·K).

The activation energy entered here for pozzolanic reactions is also assumed to influence the dissolution rate of fly ash phases (ASG and CAS_2). The default value is 100× the magnitude of the ideal gas constant, and may be used in the absence of additional information.

Step 4: Hydration behavior options

This form, shown in Figure 26, collects information on various aspects of the hydration process that have not been addressed previously.

Conversion of primary C–S–H to pozzolanic C–S–H When silica fume or other pozzolans (fly ash, etc.) are present in the starting microstructure, the user may either allow or prohibit the conversion of primary C–S–H hydration product to pozzolanic C–S–H. Pozzolanic C–S–H has a lower Ca/Si ratio (which causes extra CH to form when the primary C–S–H converts to the pozzolanic form) and a different molar volume from that of the primary C–S–H. The default condition is to prohibit the conversion of primary C–S–H. Please refer to the CEMHYD3D User's Manual [1] for more information.

Precipitation of CH on aggregate surfaces If the microstructure contains an aggregate slab (see Section 2.2.2) the user may allow CH to precipitate directly on its surfaces. This will tend

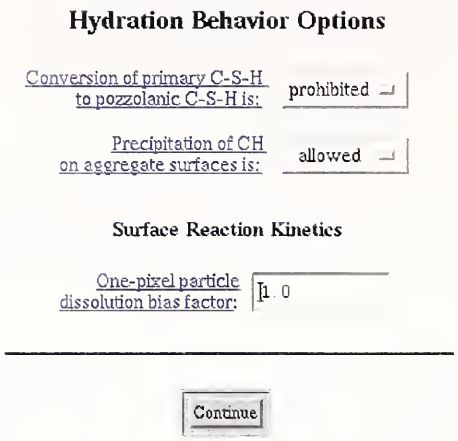


Figure 26: Fourth of five forms for launching the VCCTL hydration model (top portion).

to significantly increase the CH volume fraction immediately adjacent to the aggregate surface, and will consequently decrease the capillary porosity in this region. Because this specific aspect of the interfacial transition zone (ITZ) microstructure is still somewhat controversial, the user has the option of activating this precipitation or prohibiting it (the default being to allow the precipitation). Please consult Refs. [18, 19] for additional information.

One-pixel particle dissolution bias The probability of dissolution of one-pixel particles, regardless of their phase, can be increased using this parameter. It may be sensible to increase the bias if in the initial microstructure there are a substantial number of particles with diameters smaller than the system resolution. All such particles are assigned a diameter equal to the system resolution, so their higher reactivities will not be captured unless the bias is increased. Allowed values are in the range from 1.0 (no bias) to 100.

Step 5: Data output

This form, shown in Figure 27, is used to specify how frequently (in cycles) certain properties are evaluated and written to data files.

Evaluate percolation of porosity ... Percolation properties like this one tend to be time consuming because they involve nested iterations over most or all of the system pixels. Therefore, it is recommended that percolation properties not be evaluated every cycle. The default value of 5 is large enough that performance is not significantly affected and yet low enough that percolation thresholds can still be resolved in the data.

Evaluate percolation of total solids ... See the discussion in the previous paragraph.

Evaluate individual particle hydration ... The hydration model can keep track of the fraction of anhydrous phase reacted for each particle in the microstructure.

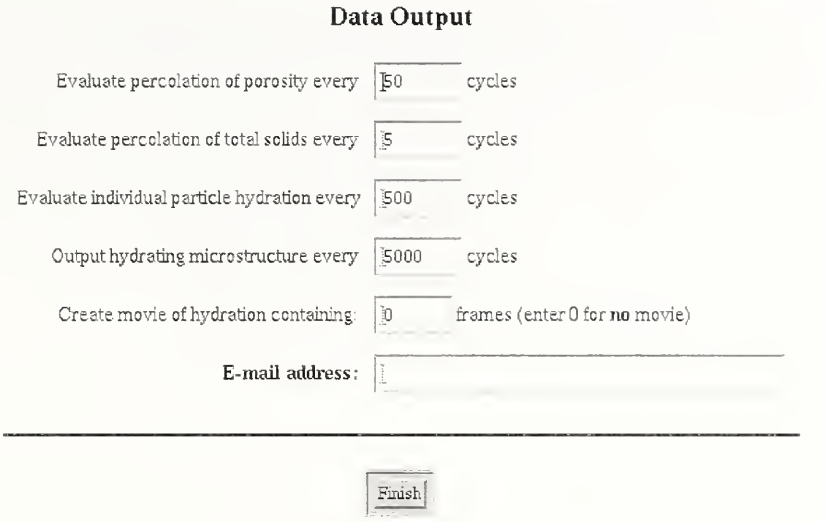


Figure 27: Fifth of five forms for launching the VCCTL hydration model.

Output hydrating microstructure ... The exact state of the entire microstructure can be saved at regular intervals during the hydration process. Although this can be helpful in preserving all the information about the course of microstructure development, keep in mind that each stored file requires between 1 and 8 Mb of storage.

Create movie of hydration ... A positive integer n entered here will cause a 2-D slice of the microstructure to be stored in a file, such that n frames are created by the end of the simulation. The hydration model then automatically creates an animated GIF file that can be viewed afterward. Consult Section 2.4.10 for details on viewing.

E-mail address The program `disrealnew` that performs hydration may take anywhere from several minutes to several hours. The actual time to completion depends on the number of cycles requested, the speed of the processor, and also depends on the size (total number of pixels) of the starting microstructure image. The VCCTL will automatically send a note to the e-mail address provided when execution completes. If no e-mail address is supplied, then a note will not be generated.

NOTE: The VCCTL is set up to perform up to two hydration simulations concurrently. Therefore, if the system is busy with two concurrent hydration simulations when another request is submitted, the user will be notified to resubmit the request at a later time.

2.3.5 Description of output file names and their contents

During hydration, several output files are created automatically. All of these files are named according to the convention:

```
fileroot.[...].N.T0.abc
```

where `fileroot` is the name of the initial microstructure file without the `.img` extension, `N` is the total number of hydration cycles, `T0` is the initial temperature, the remaining flags `a`, `b`, and `c` take on the following values:

$$\texttt{a} = \begin{cases} 0 & \text{if C–S–H conversion is prohibited.} \\ 1 & \text{if C–S–H conversion is allowed} \end{cases}$$

$$\texttt{b} = \begin{cases} 0 & \text{under isothermal conditions,} \\ 1 & \text{under adiabatic conditions,} \\ 2 & \text{under temperature-defined conditions.} \end{cases}$$

$$\texttt{c} = \begin{cases} 0 & \text{under saturated curing,} \\ 1 & \text{under sealed curing} \end{cases}$$

The string [...] represents the data that are stored in the file, and may have any of the following values

`img`	–	microstructure image file after the hydration
`heat`	–	degree of hydration (both volume and mass bases), heat released, and gel-space ratio [20], all as a function of time
`adi`	–	system temperature as a function of time
`chs`	–	chemical shrinkage as a function of time
`pha`	–	phase volumes, in pixels, as a function of time
`pps`	–	results for the examination of the percolation of the water-filled capillary porosity vs. cycles, hydration time, and degree of hydration
`pts`	–	results for the examination of the percolation of the total solids vs. cycles, computed hydration time, and degree of hydration
`phr`	–	results for the hydration degree of individual particles after specific numbers of hydration cycles

When the final hydration form is submitted, all of the user input parameters are echoed back in a form, along with the names of all of the output files that may be created by the CEMHYD3D program. Normally, however, users don't need to concern themselves with the contents of these files, as they can instead use utilities in the **Analysis submenu** (see Section 2.4) to plot any specific property of interest for the systems that have been hydrated.

2.4 Analysis submenu

This menu provides access to utilities for computing various properties of microstructures, for viewing images or movies of microstructures, and for viewing the results of various calculations that are performed by VCCTL models. The submenu is shown in Figure 28.

2.4.1 Phase statistics

This item can be selected to compute the volume pixel counts and surface pixel counts of each phase present in any 3-D microstructure. This menu selection can be employed after any step

Figure 28: The Analysis submenu selections.

during the creation of an initial microstructure, after hydration of an initial microstructure, or after degradation/leaching of a hydrated microstructure. To use this selection, the user need only supply the name of the 3-D microstructure image file to be analyzed. Within a couple minutes of submitting the form, a table of the volume and surface counts, such as that shown in Figure 29, will be displayed. Incidentally, compare the values for the clinker compounds in Figure 29 with the target values specified for this microstructure in Fig 12. In general, the target values will be matched by the distribution program to within 1 % to 2 %.

Phase Statistics for cem140wc40a.img

Thu Jan 2 10:17:23 2003

Phase	Phase ID	Volume Count	Surface Count	Volume Fraction	Surface Fraction	Mass Fraction
Porosity	0	642027	0			
C_3S	1	230897	234166	0.68617	0.68812	0.67875
C_2S	2	54750	40255	0.16270	0.11829	0.16474
C_3A	3	27178	38095	0.08077	0.11195	0.07554
C_4AF	4	23677	27783	0.07036	0.08164	0.08098
Total		336502	340299			
Gypsum	5	21471	14569			
Hemihyd.	6	0	0			
Anhydrite	7	0	0			
Pozzolan	8	0	0			

Figure 29: Phase statistics table generated using the **Phase statistics** submenu.

2.4.2 ITZ characteristics

Given a microstructure with a slab of aggregate included, this selection can be used to analyze the phase fractions present as a function of distance from the aggregate surfaces. The user supplies the name of the microstructure to be analyzed. A file with with the same root name as the microstructure file, but with the extension `.agg` instead of `.img`, filename is created. This file contains the quantitative phase counts, in pixels, as a function of distance away from the aggregate surfaces. All solid phases are examined, in addition to saturated porosity and empty porosity. All of the phases and their corresponding integer IDs are tabulated in Appendix B. In addition, if the user provides their e-mail address, this same file will be sent to the e-mail address. The data in the file then can be further analyzed or plotted using whatever software the user prefers.

2.4.3 Connectivity (Percolation)

This submenu item can be selected to evaluate the percolation properties of one or more phases in a microstructure image. The user supplies the name of the microstructure file to be evaluated and selects the phase(s) from a pull-down menu. In Version 1.1, the percolation properties of the following phases can be evaluated: saturated porosity, total porosity, CH, C–S–H, pozzolanic C–S–H, total C–S–H, ettringite, or stratlingite. An example of the results for a percolation evaluation of saturated porosity in a microstructure, named `cem140wc40a.img`, is provided in the table shown in Figure 30. For each of the three principal directions (x, y, and z), the VCCTL returns the total number of pixels of the phase of interest, the fraction of these pixels which are part of connected pathways through the microstructure, and the fraction of the total pixels which are accessible from one face of the microstructure. For the example shown in Figure 30, since no hydration has yet occurred, the initial water-filled porosity between cement particles is highly percolated, with nearly all of the water-filled porosity pixels being part of a percolated pathway.

Percolation of saturated porosity in cem140wc40a.img

Thu Jan 2 13:52:45 2003

Direction	Total Count	Percolated Fraction	Accessible Fraction
X	642027	0.9998	0.9998
Y	642027	0.9997	0.9998
Z	642027	0.9998	0.9998

If the table above displays nothing or all zeros, press the **Reload** button on your web browser

Figure 30: Evaluation of percolation using the **Connectivity (Percolation)** submenu item.

2.4.4 Results of hydration simulation

This option is used both to plot the different predicted properties and to enter experimental data for comparison against the predicted values. Upon making this selection, a form is displayed with two pull-down menus to select a specific system for which either (1) to list the available plots or (2) to enter a set of experimental data, as shown in Figure 31. The form is submitted by clicking the left button in either row ("List data files for plotting" or "List data files for data entry").

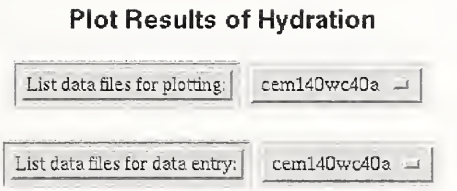


Figure 31: Pull-down menus to select a hydrated system for either plotting properties or entering experimental data.

Upon submission of the form, a second form, containing a table of the various options available either for plotting or data entry, is displayed (see Figure 32 for an example of a portion the table returned in the case of plotting).

Plot Selection Form

Case: cem140wc40a

Create All Plots Include data: Strength prefactor: 95 MPa Strength exponent: 2.6	Plot Type	Number of Cycles	Pozz. CSH Conversion	Heat Transfer Mode	Curing	Initial Temperature
Create Plot	adiabatic heat signature	100	off	isothermal	saturated	20
Create Plot	adiabatic heat signature	2000	off	isothermal	saturated	20
Create Plot	adiabatic heat signature	2001	off	isothermal	saturated	20
Create Plot	chemical shrinkage	100	off	isothermal	saturated	20

Figure 32: Top portion of table for plotting hydration properties.

With this table, in the case of plotting, the user can select to create all available plots for a given system, or simply to create a single plot of interest. In all cases, the user can elect to include the experimental data (when available) on the plot. Typically, the computer model data is plotted using blue squares connected by a blue line, while the experimental data is shown as discrete red diamond-shaped points. The plot is typically labelled with the name of the datafile from which it was created.

In Version 1.1 of VCCTL, the following plots are available (when the appropriate data have been created during a hydration run):

heat signature:	system temperature vs. computed hydration time (not very interesting for hydration under isothermal conditions)
chemical shrinkage:	chemical shrinkage (ml/g cement) vs. computed hydration time (h)
hydration:	degree of hydration (mass basis) vs. computed hydration time
heat release:	cumulative heat release (kJ/kg cement) vs. computed hydration time
compressive strength:	estimated compressive strength (MPa) vs. computed hydration time. The user must provide a pre-factor to be used in the calculation of compressive strength based on Power's gel-space ratio theory [20]
capillary pore percolation:	connected capillary porosity vs. either total porosity or computed hydration time
solids percolation:	connected "total solids" vs. either computed hydration time or degree of hydration

To enter experimental data corresponding to a specific system, the user has the option of (1) downloading the data into the VCCTL from a datafile **located on the client computer** or (2) entering the data manually. In the latter case, the VCCTL will provide a fill-in table with two columns corresponding to the values to be plotted on the x-axis and y-axis, respectively. For example, to enter data for adiabatic heat signature, the user would have to enter the time-temperature results into this table and then simply submit the form (using the "Copy data" button above the data entry table) to store this data file for later access during plotting. Always, when experimental data have been entered, the user has the option of including the data file, or omitting it, in the associated plot of simulation results.

2.4.5 Results of sulfate attack

This feature is currently under development within the Virtual Cement and Concrete Testing Laboratory Consortium.

2.4.6 Results of elastic moduli calculation

This feature is currently under development within the Virtual Cement and Concrete Testing Laboratory Consortium.

2.4.7 Results of DC conductivity calculation

This feature is currently under development within the Virtual Cement and Concrete Testing Laboratory Consortium.

2.4.8 View a 2-D slice of a 3-D microstructure

This selection enables the user to graphically examine a 2-D slice from any existing 3-D microstructure (starting, hydrated, leached, etc). The user simply supplies the name of the image to be displayed, the z-plane (slice) to select from the 3-D microstructure, and a magnification factor ($1\times$ to $10\times$) for viewing the image. The VCCTL will locate the proper slice of the selected image and display a 2-D color image of the microstructure, along with a key identifying the phases corresponding to each color. An example is shown in Figure 33.

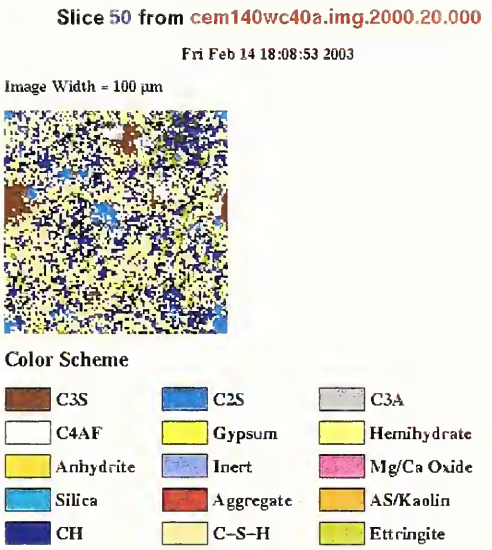


Figure 33: Display of a 2-D slice from a 3-D microstructure.

If this selection is used repeatedly with the same 3-D image filename, depending on the user's Internet browser settings and preferences, the "Reload" or "Refresh" button on the web browser may need to be pressed to update the displayed image to be the currently selected one. In the extreme cases where this button doesn't load the newly generated image, the user will need to restart their Internet browser or use some other measure to force it to empty the previous image from its cache.

2.4.9 Generate animated scan or hydration movie

An alternate method of viewing a microstructure is to create a fly-through scan—one z-plane slice at a time—of the 3-D image. This selection can be used to create an animated GIF file for a user-specified 3-D microstructure. For this selection, the user supplies the following information before submitting the displayed form:

- the name of the microstructure to be animated,
- a new filename in which to store the animated GIF file,
- the number of 2-D slices to include in the animation (from 1 up to the system size), and
- the magnification ($1\times$–$10\times$) to use.

The first slice of the microstructure is always used as the starting slice for the 3-D animation generation. Typically, to generate a complete (100 slice) animation of a 3-D microstructure will require up to 20 min of CPU time. Therefore, the user should wait at least that long before trying to view the animation using the next submenu selection.

NOTE: The VCCTL is set up to create only one animation at any specific time. Therefore, if the system is busy creating one animation when another request is submitted, the user will be notified to resubmit the job at a later time.

2.4.10 View animated scan or hydration movie

This item is used simply to view the animated GIF files created using the previous submenu item. The user need only supply the name of the animated GIF file to be displayed. The animated GIF file will be looped five times from start to finish.

2.4.11 View a data file

This feature is currently under development within the Virtual Cement and Concrete Testing Laboratory Consortium.

2.5 Transport Properties

This submenu enables the user to estimate the transport properties (i.e., diffusion coefficient of a particular ionic species) of a concrete, or to calculate directly the diffusion coefficient of a cement paste microstructure that was created, and hydrated and/or degraded using VCCTL models. It should be recognized that the diffusion coefficient is a difficult quantity to calculate with accuracy, because it depends on complicated aspects of the pore solution composition, in addition to the state of the microstructure [21]. A much simpler quantity to calculate, and one which directly reflects the influence of microstructure on ionic tansport, is the formation factor.

2.5.1 Estimate chloride ion diffusivity of a concrete based on mixture parameters

This submenu selection is provided to estimate a chloride-ion diffusion coefficient for a concrete (which may contain silica fume), based on knowledge of its mixture proportions and the degree of hydration of the cement binder. The equations used to make the estimate have been presented previously [22], are based on a regression performed using published data, and are also incorporated into a prototype Computer Integrated Knowledge System (CIKS) for predicting the service life of steel-reinforced concrete exposed to chloride ions [23], available separately from the VCCTL.

To use this submenu selection, the user supplies the following four mix parameters for the concrete of interest (see Figure 34): the w/c ratio, the silica fume content (mass % on a cement basis), the volume fraction of aggregates, and the degree of hydration of the cement. **Recommended ranges of applicability for each of these parameters are provided on the fill-in form; extrapolations beyond these ranges should be made only with caution.**

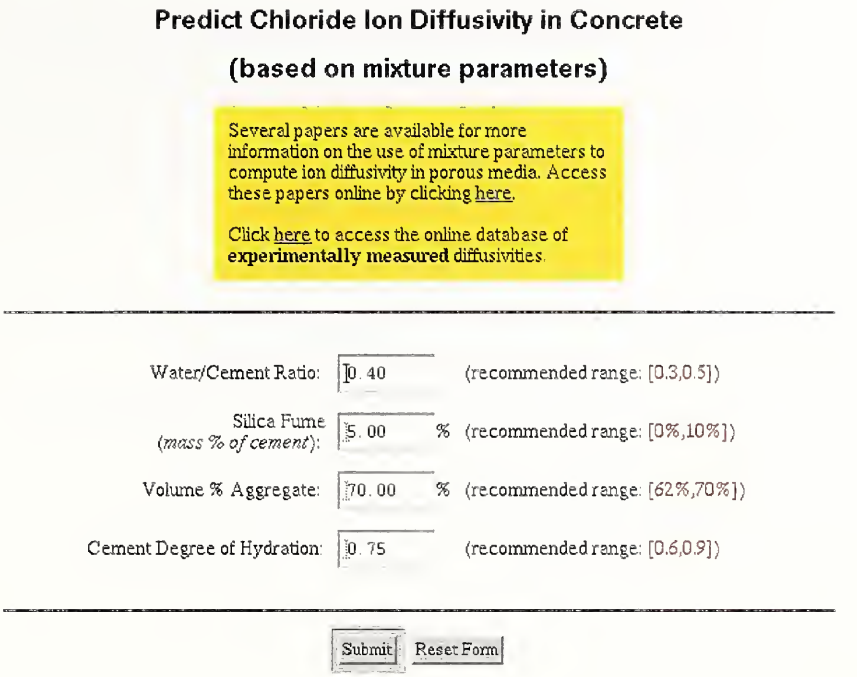


Figure 34: Form for entering mixture parameter data used to estimate the chloride-ion diffusion coefficient of concrete.

After the form is submitted, the estimated value of the diffusion coefficient, D, (in m^2/s) is returned along with the 90 % confidence limits for D and some recommendations on methods to lower the value of D, if desired (see Figure 35 for an example of the output).

2.5.2 Compute DC conductivity

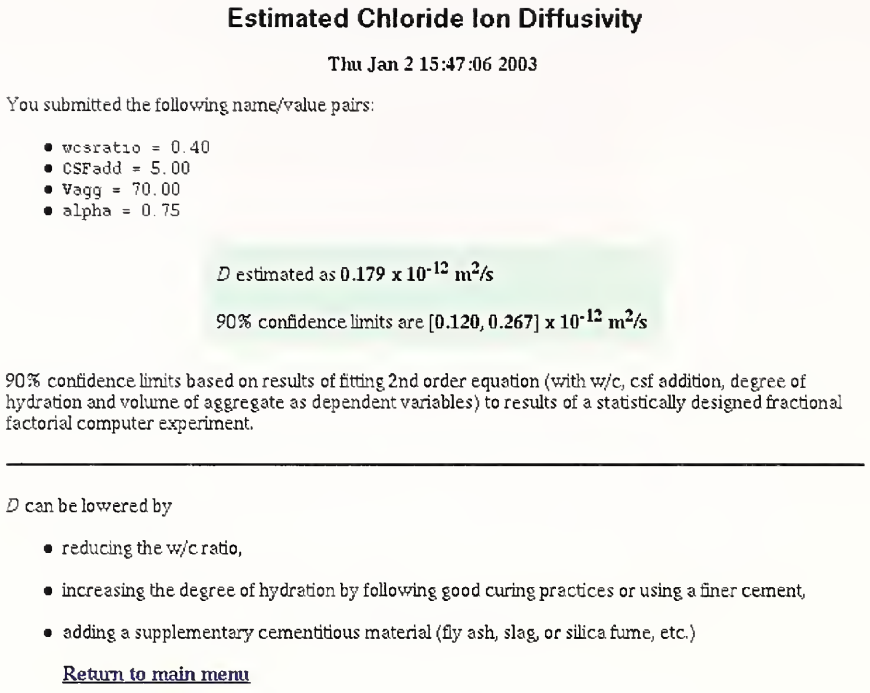
This feature is currently under development within the Virtual Cement and Concrete Testing Laboratory Consortium.

2.6 Rheology

This feature is currently under development within the Virtual Cement and Concrete Testing Laboratory Consortium.

2.7 Elastic Properties

This feature is currently under development within the Virtual Cement and Concrete Testing Laboratory Consortium.



Estimated Chloride Ion Diffusivity

Thu Jan 2 15:47:06 2003

You submitted the following name/value pairs:

- wcsratio = 0.40
- CSFadd = 5.00
- Vagg = 70.00
- alpha = 0.75

D estimated as **0.179 x 10^{-12} m^2/s**

90% confidence limits are **[0.120, 0.267] x 10^{-12} m^2/s**

90% confidence limits based on results of fitting 2nd order equation (with w/c, csf addition, degree of hydration and volume of aggregate as dependent variables) to results of a statistically designed fractional factorial computer experiment.

D can be lowered by

- reducing the w/c ratio,
- increasing the degree of hydration by following good curing practices or using a finer cement,
- adding a supplementary cementitious material (fly ash, slag, or silica fume, etc.)

Return to main menu

Figure 35: Example of an output page generated when the chloride-ion diffusion coefficient of concrete is estimated based on mixture parameters.

2.8 Degradation

Any assessment of durability depends on knowledge of the mechanism(s) by which degradation occurs. In VCCTL Version 1.1, degradation by **leaching** can be simulated. A model for degradation by **magnesium sulfate attack** is under development within the Virtual Cement and Concrete Testing Laboratory Consortium, and should be available in upcoming versions.

2.8.1 Leach CH/cement

This option can be used to selectively leach (remove) a portion or the complete volume of one or more phases from a hydrated microstructure. The calcium hydroxide (CH) and the initial four cement clinker phases all can be leached, and the user selects which phases to include in a specific execution of the algorithm.

The input form for the leaching simulation is shown in Figure 36. The fields are:

Random number seed The user must enter a *negative integer* (in the range [-32767,-1]) in this field. See the description in Section 2.2.2 for more information on the purpose of random number seeds in VCCTL.

Microstructure to leach The user must supply the file name of the microstructure to be leached, complete with any extensions.

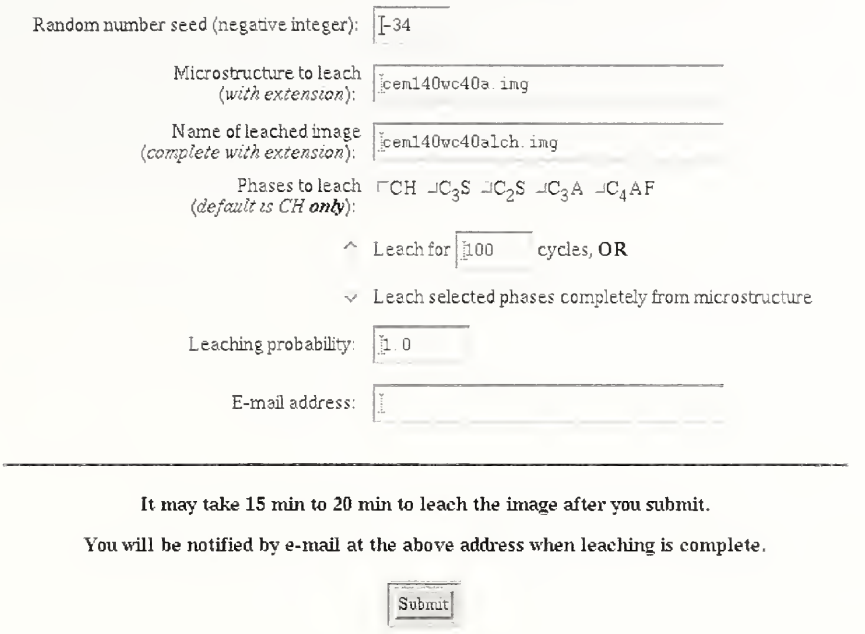


Figure 36: Form for launching a simulation of leaching of one or more phases from a cement paste microstructure.

Name of leached image A new file name, in which to store the microstructure after leaching, must be provided. If the file name already exists, the user will be notified and asked to specify a different file name.

Phases to leach Currently, the user can select to leach any combination of the following phases from a cement paste microstructure: CH, C_3S, C_2S, C_3A, and C_4AF. The default is to leach only CH.

Termination of leaching Two options are available:

1. Leach for a specified number of cycles (default 100)
2. Leach the selected phases completely from the microstructure

If the first option is selected, then leaching proceeds by the specified number of reaction cycles, progressing from the exterior of the microstructure inward. The reaction probability is specified by the user (see the next entry). If the second option is selected, then the microstructure is scanned once and all pixels of the user-specified phase(s) are converted to saturated porosity.

Leaching probability If the user chooses to leach for a defined number of cycles, then a leaching probability (p_l in the range 0.0-1.0), is required in this field.

E-mail address The program `leach3d` that performs the leaching simulation may take several minutes to complete. The VCCTL will automatically send a note to the e-mail address provided when execution completes. If no e-mail address is supplied, then a note will not be generated.

NOTE: The VCCTL is set up to perform only one leaching simulation at any specific time. If the system is already executing `leach3d` for one microstructure when another request is submitted, the user will be notified to resubmit the request at a later time.

2.9 Documentation

The Documentation submenu contains further information about the Virtual Cement and Concrete Testing Laboratory, including links to

- this User's Guide
- the NIST Electronic Monograph
- a Frequently Asked Questions (FAQ) repository
- a list of NIST personnel who are involved in VCCTL research

3 Summary

A detailed description of the web-based menu-driven interface to Version 1.1 of the VCCTL has been provided. The interface consists of a series of fill-in HTML forms that allow the user to specify input parameters for, execute, and view the results of various component programs of the VCCTL. The user is notified of the completion of program execution and, in a few cases, is sent a copy of the analysis results by e-mail. The system has been designed to bring the VCCTL to the user's desktop computer, where a standard Internet browser provides a powerful connection to the world of virtual design, analysis, and optimization of cement-based materials.

4 Acknowledgments

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A Appendix A

This appendix provides an example of how to create a blended (or composite) cement that is ready to be subjected to a simulation of hydration. As will become evident, careful consideration of the mix design is warranted before "jumping in" to the VCCTL menus.

A.1 Mix design

- CCRL Cement 140 with 5 % (by volume) total calcium sulfate, with the calcium sulfate being 80 % dihydrate and 20 % hemihydrate. Assume PSD of calcium sulfate phases is the same as that of the cement.
- Fumed silica, 4 % of the total solid mass
  - PSD to be approximated as uniform 3 μm spheres
- Fly Ash, 15 % of the total solid mass
- PSD assumed to be bimodal, sharply peaked around 5 μm and 25 μm.
- Phase composition: 33 % aluminosilicate glass, 39 % SiO_2, 28 % inert (on a volume basis)
- Morphology: predominantly monophase spheres.
- Total water-solids ratio is to be 0.5

From this information, we can calculate the numbers of pixels of each generic type of component needed (cement, silica fume, and fly ash).

A.2 Calculation of target pixel numbers

First, we need to know the fraction f_s of the system pixels that should be solid. After some algebra, the following formula can be derived:

$$f_s = \frac{1}{1 + (\mathrm{w/s}) \cdot \rho_s} \tag{4}$$

where w/s is the water-solids ratio (0.5 in this example) and ρ_s is the specific gravity of the solids, which in this case must be taken as a weighted average over all of the solid phases as follows:

$$\rho_s = \rho_{\mathrm{ref}} + \sum_{i-1}^{k-1} f_i \left(\rho_i - \rho_{\mathrm{ref}}\right) \tag{5}$$

where ρ_{ref} is the specific gravity of a phase chosen as a reference. In Eq. (5), it is assumed that there are k solid phases, and that the i-th phase has specific gravity ρ_i and volume fraction f_i (fraction of the total solids, not the system). The sum is taken over all the phases except the reference phase. For this example, we are requiring that the **mass fraction** of fumed silica is 0.04, that of fly ash

is 0.15, and that of the cement (clinker plus gypsum) is 0.81. Therefore, we need to convert mass fractions to volume fractions. For each component $i > 1$, this gives an equation of the form

$$f_i = \frac{\chi_i \rho_s}{\rho_i} = \frac{\chi_i}{\rho_i} \left(\rho_1 + \sum_{j=2}^{k} f_j \left(\rho_j - \rho_1 \right) \right) \tag{6}$$

Again, for this example, $k = 3$, and we take the cement (clinker plus gypsum) as the reference "phase". Examination of the previous equation reveals that we must know the specific gravity of the cement (plus gypsum). We calculate this using an equation like Eq. (5):

$$\rho_{\text{cement}} = \rho_{\text{clinker}} + f_{\text{gyp}} \left(\rho_{\text{gyp}} - \rho_{\text{clinker}} \right) + f_{\text{hemi}} \left(\rho_{\text{hemi}} - \rho_{\text{clinker}} \right) \tag{7}$$

Our mix design dictates $f_{\text{gyp}} = 0.04$ and $f_{\text{hemi}} = 0.01$. Furthermore, examination of Table 1 gives $\rho_{\text{clinker}} = 3.2$, $\rho_{\text{gyp}} = 2.32$, and $\rho_{\text{hemi}} = 2.73$. Therefore, substitution into the previous equation gives $\rho_{\text{cement}} = 3.16$.

Next, for this example Eq. (6) expands to the following coupled equations, where we substitute $\rho_1 = \rho_{\text{cement}} = 3.16$:

$$f_{\text{FS}} = \frac{\chi_{\text{FS}}}{\rho_{\text{FS}}} \left(3.16 + f_{\text{FS}} (\rho_F S - 3.16) + f_{\text{FA}} (\rho_{\text{FA}} - 3.16) \right) \tag{8}$$

$$f_{\text{FA}} = \frac{\chi_{\text{FA}}}{\rho_{\text{FA}}} \left(3.16 + f_{\text{FS}} (\rho_F S - 3.16) + f_{\text{FA}} (\rho_{\text{FA}} - 3.16) \right) \tag{9}$$

where subscript FS denotes fumed silica and FA denotes fly ash. Substituting in the values from Table (1) and the mass fractions required by the mix designs gives

$$f_{\text{FS}} = 0.050 \tag{10}$$

$$f_{\text{FA}} = 0.182 \tag{11}$$

$$f_{\text{cement}} = 1 - f_{\text{FS}} - f_{\text{FA}} = 0.768 \tag{12}$$

We may now substitute these values into Eq. (5) to find the average solid specific gravity:

$$\begin{aligned} \rho_s &= \rho_{\text{cement}} + f_{\text{FS}} \left(\rho_{\text{FS}} - \rho_{\text{cement}} \right) + f_{\text{FA}} \left(\rho_{\text{FA}} - \rho_{\text{cement}} \right) \\ &= 3.16 + 0.05(2.2 - 3.16) + 0.182(2.55 - 3.16) \\ &= 3.00 \end{aligned} \tag{13}$$

And, having a value for ρ_s, we may substitute into Eq. (4) to find the volume fraction of solids in the system. With w/s = 0.5 from the mix design, Eq. (4) gives $f_s = 0.4$. Thus, because there are 1M (one million) pixels in the system (100 pixels in each dimension), the target for the total number of solid pixels shall be 0.4M. Therefore, immediately we may derive the number of pixels needed for fumed silica and fly ash,

$$N_{\text{FS}} = 1 \times 10^6 \cdot f_s \cdot f_{\text{FS}} = 20000 \tag{14}$$

$$N_{\text{FA}} = 1 \times 10^6 \cdot f_s \cdot f_{\text{FA}} = 72800 \tag{15}$$

$$N_{\text{cement}} = 400000 - 20000 - 72800 = 307200 \tag{16}$$

Finally, with this information for the numbers of each type of generic particle, we may begin to create the three PSD files that are required.

A.3 Creating the PSD files

A.3.1 Cement

To create the cement PSD file, enter the **Build Microstructure** menu and click on the **Create a PSD file** submenu (see Section 2.2.1). Choose "cement140" from the pull-down menu for CCRL Cement 140. Click "Submit ", and when the next page is displayed, scroll down to the form entry for **Total number of pixels**. Enter `307200` in the field and then click anywhere outside that field. The Javascript automatically calculates the number of particles of each size. After it has completed, the total number of pixels has changed to `307210`. This value is within 0.003 % of the target value, so we will accept it and save the file by entering as `excement` in the **PSD file to create** field below (see Fig. 37). Pressing "Submit" will save the file as `excement.psd`

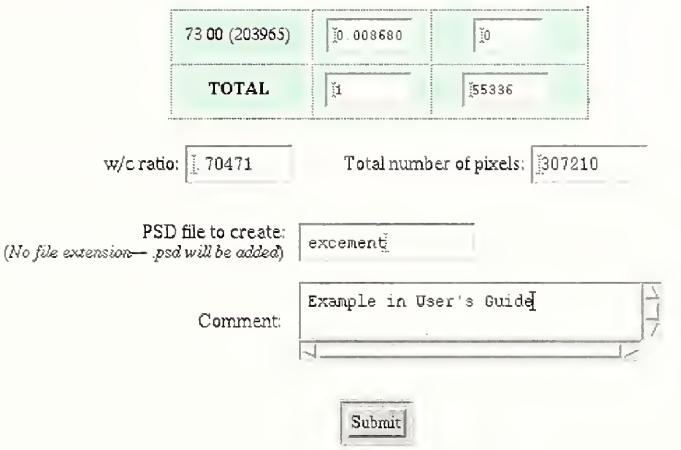

Figure 37: PSD form for creating example cement PSD file.

A.3.2 Fumed Silica

Again click on the **Create a PSD file** submenu (Section 2.2.1). This time, it does not matter which cement is chosen from the pull-down menu because we will modify the mass fractions such that only 3 μm particles are created. This time, as already mentioned, manually enter `0.0` for all the mass fractions in the table **except** that for 3 μm, which should be changed to `1.0`. Next, enter a value of `20000` in the field for **Total number of pixels** and click anywhere outside that field. The Javascript now determines that there should be 1053 particles of size 3 μm, and because each of these particles is comprised of 19 pixels, this sums to 20007 pixels, within 0.04 % of the target. (see Figure 38). Save this file as `exfs.psd` by entering `exfs` in the **PSD file to create** field, and press "Submit".

A.3.3 Fly Ash

Again click on the **Create a PSD file** submenu (Section 2.2.1). Once again, it does not matter which cement is chosen from the pull-down menu because we will modify the mass fractions such that only 5 μm and 25 μm particles are created. Press "Submit". This time, manually enter `0.0` for all the mass fractions in the table **except** that for 5 μm, which should be changed to `0.2`, and

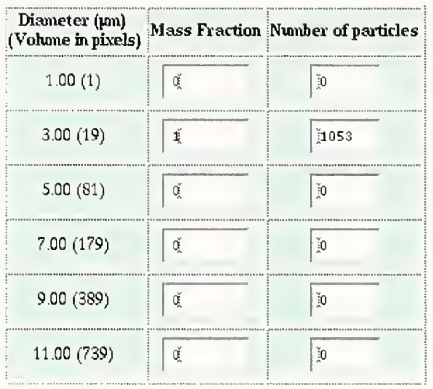

Figure 38: PSD form for creating example fumed silica PSD file.

that for 25 μm, which should changed to `0.8`. Next, enter a value of `72800` in the field for **Total number of pixels** and click anywhere outside that field. This time, Javascript now determines that there should be 196 total fly ash particles, seven having diameter 25 μm and the remainder having diameter 5 μm. The total number of pixels is 72828, which is within 0.04 % of the desired value. Save this file as `exfa.psd` by entering `exfa` in the **PSD file to create** field, and press "Submit".

A.4 Making the "generic" microstructure

Click on the **Generate initial microstructure** submenu (Section 2.2.2) of the **Build Microstructure** menu. Because we will be creating the microstructure from existing PSD files, click the button labeled "Read particle sizes from file(s)". We will choose to **not** add an aggregate particle, and we will also **not** select flocculation. The dispersion distance will be kept at its default value of zero (pixel units).

A.4.1 Sulfate additions

Recall that the mix design in this example requires 5 % calcium sulfate by volume, with 80 % of it being the dihydrate form and 20 % being the hemihydrate form. Therefore the three text boxes should be filled with `0.05`, `0.20`, and `0.00`, respectively, as shown in Figure 39.

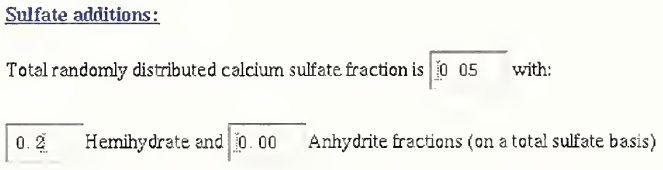

Figure 39: Values for sulfate additions based on example mix design.

For the particle size distribution files, enter `excement.psd`, `exfs.psd`, and `exfa.psd` in the fields for Cement, Pozzolan, and Fly Ash, respectively. Save the microstructure as `example.img` by entering `example` in the **Name this microstructure** field, and press "Submit".

A.5 Distributing the cement phases

The next step is to distribute the four major clinker phases among all the generic cement particles. To do this, click on the **Distribute cement phases** submenu (Section 2.2.3) in the **Build Microstructure** menu. Because we are trying to model CCRL Cement 140 in this example, select "cement140" from the pull-down menu. Press "Submit".

In the next form that is displayed, scroll down to the main part of the form. Enter a negative random number if desired, or just accept the default number. In the next field, enter `example.img` as the initial microstructure file (the one just created in the previous step). For an output microstructure image file, enter `examplea`. The numbers in the table are automatically loaded from the database for CCRL Cement 140, so there is no need to adjust them. Enter your e-mail address in the appropriate field. Print this form from your browser, or record the volume fractions and surface area fractions for later comparison, and then press "Submit". The calculation should take 20–60 min.

A.6 Checking the volume fractions and surface fractions

It is generally good practice to check that the distribution of clinker phases produced satisfactorily accurate results for the volume fractions and surface fractions of the clinker phases. Click on the **Phase statistics** submenu (Section 2.4.1) in the **Analysis** menu, enter `examplea.img` (the **output** file from the previous step) in the text field that appears, and press the "Submit" button. The volume fractions and surface fractions for the four major clinker phases are displayed near the top of the table that is displayed. The values should agree to within a few parts in the third decimal place.

A.7 Distributing the fly ash phases

The final step in this example will be to distribute the fly ash phases amongst the generic fly ash particles. Click on the **Distribute fly ash phases** submenu (Section 2.2.6) in the **Build Microstructure** menu. Enter a random number or accept the default value.

Because the mix design specifications in the example suggest that each particle is composed of one phase predominantly, we will elect to distribute the fly ash phases randomly on a **particle** basis, by selecting the radio button next to that option. The initial microstructure file is `examplea.img` (the output file from distributing the clinker phases). The particle image file should be the name of the **generic** microstructure image (in this case `example.img`) except with a "p" as the first character. Enter `pexample.img` in this field. The new microstructure file name should be `exampleb.img` so enter `exampleb` in the field for **New microstructure file name**. Recall from earlier in the example that the number of generic fly ash pixels is 72828; enter this number for **Number of fly ash pixels**.

The mix design in this example specifies that the fly ash is composed of 33 % aluminosilicate glass, 39 % silica, and 28 % inert filler. Therefore, enter 0.33 and 0.39 in the aluminosilicate glass and silica table rows, respectively, and make sure all the others are set to zero. The remainder will be assigned as inert filler automatically. Print out the form for future records, and then press the

"Submit" button. The computation should take only a few moments, so there is little need to enter an e-mail address.

B Appendix B

Phase	ID	Phase	ID
Saturated porosity	0	Ettringite	19
C_3S	1	Fe-stabilized Ettringite	20
C_2S	2	AFm	21
C_3A	3	FH_3	22
C_4AF	4	Pozzolanic C–S–H	23
Gypsum	5	$CaCl_2$	25
Hemihydrate	6	Friedel's salt	26
Anhydrite	7	Stratlingite	27
Pozzolan	8	Secondary gypsum	28
Inert	9	Absorbed gypsum	29
Aggregate	11	Dried porosity	47
AS glass	12	Empty dry porosity	48
CAS_2	13	Empty porosity	49
C_3A (fly ash)	14		
Generic fly ash	15		
CH	16		
C–S–H	17		
C_3AH_6	18		

Table 2: Identification numbers for all phases recognized by VCCTL Version 1.1.

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